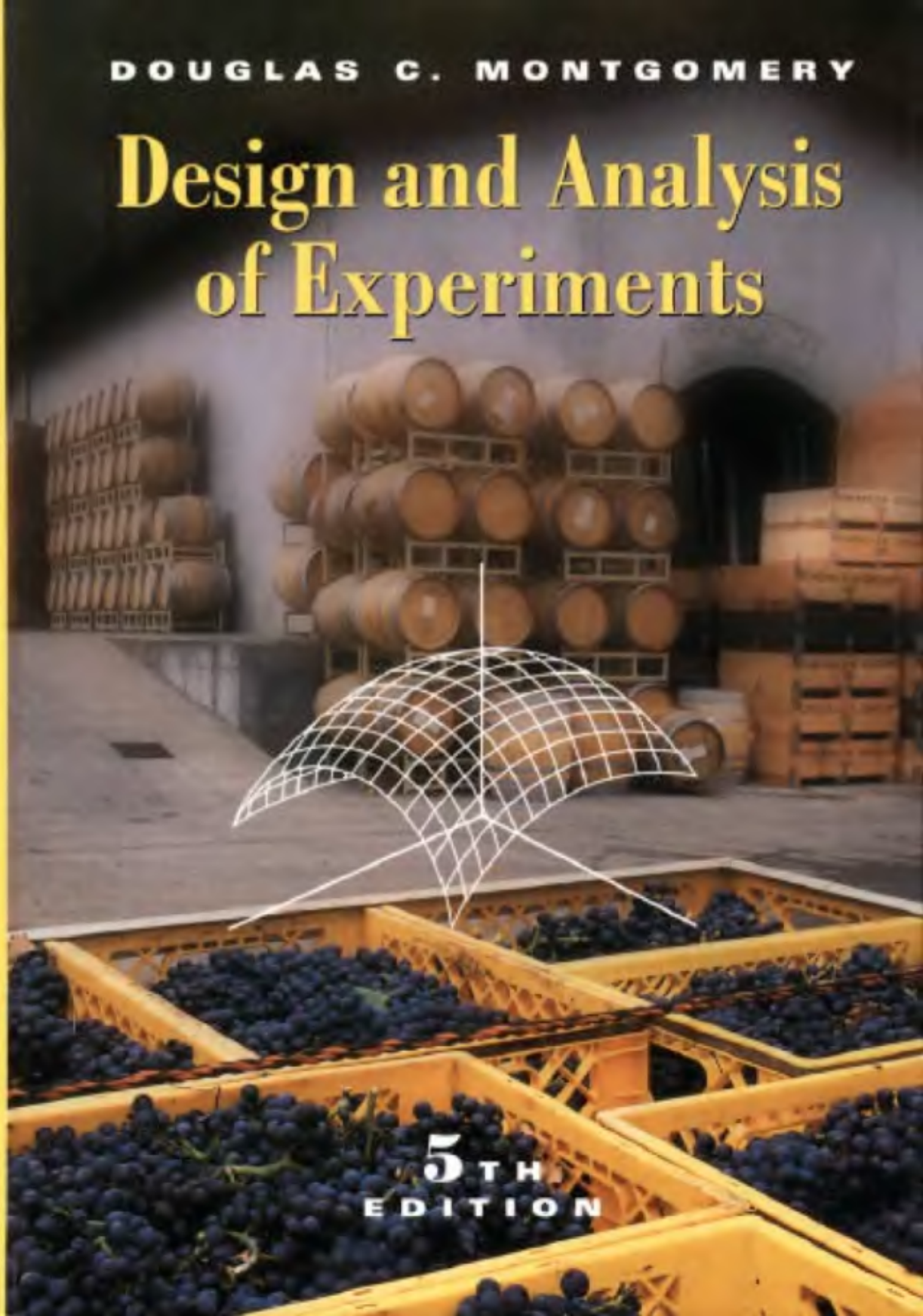
DOUGLAS C. MONTGOMERY

Design and Analysis of Experiments



5TH EDITION

DESIGN AND ANALYSIS OF EXPERIMENTS

Fifth Edition

Douglas C. Montgomery

ARIZONA STATE UNIVERSITY

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Preface

This is an introductory textbook dealing with the design and analysis of experiments. It is based on college-level courses in design of experiments that I have taught for over 25 years at Arizona State University, the University of Washington, and the Georgia Institute of Technology. It also reflects the methods that I have found useful in my own professional practice as an engineering and statistical consultant in the general areas of product and process design, process improvement, and quality engineering.

The book is intended for students who have completed a first course in statistical methods. This background course should include at least some techniques of descriptive statistics, the normal distribution, and an introduction to basic concepts of confidence intervals and hypothesis testing for means and variances. Chapters 10 and 11 require some familiarity with matrix algebra.

Because the prerequisites are relatively modest, this book can be used in a second course on statistics focusing on statistical design of experiments for undergraduate students in engineering, the physical and chemical sciences, mathematics, and other fields of science. For many years I have taught a course from the book at the first-year graduate level in engineering. Students in this course come from all the traditional fields of engineering, physics, chemistry, mathematics, operations research, and statistics. I have also used this book as the basis of an industrial short course on design of experiments for practicing technical professionals with a wide variety of backgrounds. There are numerous examples illustrating all of the design and analysis techniques. These examples are based on real-world applications of experimental design and are drawn from many different fields of engineering and the sciences. This adds a strong applications flavor to an academic course for engineers and scientists and makes the book useful as a reference tool for experimenters in a variety of disciplines.

ABOUT THE BOOK

The fifth edition is a major revision of the book. I have tried to maintain the balance between design and analysis topics of previous editions; however, there are many new topics and examples, and I have reorganized much of the material. There is much more emphasis on the computer in this edition. During the last few years a number of excellent software products to assist experimenters in both the design and analysis phases of this subject have appeared. I have included output from two of these products, Minitab and Design-Expert, at many points in the text. Minitab is a widely available general-purpose statistical software package that has good data analysis capabilities, and which handles the analysis of experiments with both fixed and random factors (including the mixed model) quite nicely. Design-Expert is a package focused exclusively on experimental design. It has many capabilities for construction and evaluation of designs and extensive analysis features. A student version of Design-Expert is available with this book, and its use is highly recommended. I urge all instructors who use this book to incorporate com-

puter software into your course. (In my course, I bring a laptop computer and an overhead display panel to every lecture, and every design or analysis topic discussed in class is illustrated with the computer.)

I have increased the emphasis on the connection between the experiment and the model that the experimenter can develop from the results of the experiment. Engineers (and physical and chemical scientists to a large extent) learn about physical mechanisms and their underlying mechanistic models early in their academic training, and throughout much of their professional careers they are involved with manipulation of these models. Statistically designed experiments offer the engineer a valid basis for developing an *empirical* model of the system being investigated. This empirical model can then be manipulated (perhaps through a response surface or contour plot, or perhaps mathematically) just as any other engineering model. I have discovered through many years of teaching that this viewpoint is very effective in creating enthusiasm in the engineering community for statistically designed experiments. Therefore, the notion of an underlying empirical model for the experiment and response surfaces appears early in the book and receives much more emphasis.

I have also made an effort to get the reader to the critical topics involving factorial designs much faster. To facilitate this, the introductory material on completely randomized single-factor experiments and the analysis of variance has been condensed into a single chapter (Chapter 3). I have expanded the material on factorial and fractional factorial designs (Chapters 5–9) in an effort to make the material flow more effectively from both the reader's and the instructor's viewpoint and to place more emphasis on the empirical model. The chapter on response surfaces (Chapter 11) immediately follows the material on factorial and fractional factorial designs and regression modeling. I have expanded this chapter, adding new material on alphabetically optimal designs, experiments with mixtures, and the robust parameter design problem. Chapters 12 and 13 discuss experiments involving random effects and some applications of these concepts to nested and split-plot designs. Chapter 14 is an overview of important design and analysis topics: nonnormality of the response, the Box–Cox method for selecting the form of a transformation, and other alternatives; unbalanced factorial experiments; the analysis of covariance, including covariates in a factorial design, and repeated measures.

Throughout the book I have stressed the importance of experimental design as a tool for practicing engineers to use for product design and development as well as process development and improvement. The use of experimental design in developing products that are robust to environmental factors and other sources of variability is illustrated. I believe that the use of experimental design early in the product cycle can substantially reduce development lead time and cost, leading to processes and products that perform better in the field and have higher reliability than those developed using other approaches.

The book contains more material than can be covered comfortably in one course, and I hope that instructors will be able to either vary the content of each course offering or discuss some topics in greater depth, depending on class interest. There are problem sets at the end of each chapter (except Chapter 1). These problems vary in scope from computational exercises, designed to reinforce the fundamentals, to extensions or elaboration of basic principles.

My own course focuses extensively on factorial and fractional factorial designs. Consequently, I usually cover Chapter 1, Chapter 2 (very quickly), most of Chapter 3, Chapter 4 (excluding the material on incomplete blocks and only mentioning Latin squares briefly), and I discuss Chapters 5 through 8 on factorials and two-level factorial

and fractional factorial designs in detail. To conclude the course, I introduce response surface methodology (Chapter 11) and give an overview of random effects models (Chapter 12) and nested and split-plot designs (Chapter 13). I always require the students to complete a term project that involves designing, conducting, and presenting the results of a statistically designed experiment. I require them to do this in teams, because this is the way that much industrial experimentation is conducted. They must present the results of this project, both orally and in written form.

THE SUPPLEMENTAL TEXT MATERIAL

For the fifth edition I have prepared supplemental text material for each chapter of the book. Often, this supplemental material elaborates on topics that could not be discussed in greater detail in the book. I have also presented some subjects that do not appear directly in the book, but an introduction to them could prove useful to some students and professional practitioners. Some of this material is at a higher mathematical level than the text. I realize that instructors use this book with a wide array of audiences, and some more advanced design courses could possibly benefit from including several of the supplemental text material topics. This material is in electronic form on the Instructor's CD/ROM and is on the World Wide Web site for this book.

WEB SITE

Current supporting material for instructors and students is available at the Web site *www.wiley.com/college/montgomery*. This site will be used to communicate information about innovations and recommendations for effectively using this text. The supplemental text material described above is available at the site, along with electronic versions of data sets used for examples and homework problems, a course syllabus, a complete set of Power Point lecture slides created by the author, and student term projects from the course at Arizona State University.

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I express my appreciation to the many students, instructors, and colleagues who have used the four earlier editions of this book and who have made helpful suggestions for its revision. The contributions of Dr. Raymond H. Myers, Dr. G. Geoffrey Vining, Dr. Dennis Lin, Dr. John Ramberg, Dr. Joseph Pignatiello, Dr. Lloyd S. Nelson, Dr. Andre Khuri, Dr. Peter Nelson, Dr. John A. Cornell, Dr. George C. Runger, Dr. Bert Keats, Dr. Dwayne Rollier, Dr. Norma Hubele, Dr. Cynthia Lowry, Dr. Russell G. Heikes, Dr. Harrison M. Wadsworth, Dr. William W. Hines, Dr. Arvind Shah, Dr. Jane Ammons, Dr. Diane Schaub, Mr. Mark Anderson, Mr. Pat Whitcomb, Dr. Pat Spagon, and Dr. William DuMouche were particularly valuable. My Department Chair, Dr. Gary Hogg, has provided an intellectually stimulating environment in which to work.

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Douglas C. Montgomery
Tempe, Arizona

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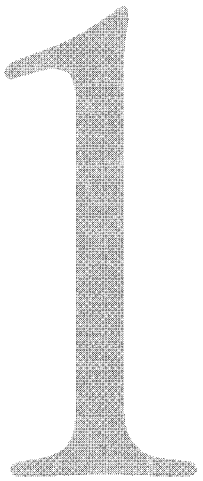


Introduction

1-1 STRATEGY OF EXPERIMENTATION

Experiments are performed by investigators in virtually all fields of inquiry, usually to discover something about a particular process or system. Literally, an experiment is a **test**. More formally, we can define an **experiment** as a test or series of tests in which purposeful changes are made to the input variables of a process or system so that we may observe and identify the reasons for changes that may be observed in the output response.

This book is about planning and conducting experiments and about analyzing the resulting data so that valid and objective conclusions are obtained. Our focus is on experiments in the engineering, physical, and chemical sciences. In engineering, experimentation plays an important role in new product design, manufacturing process development, and process improvement. The objective in many cases may be to develop a **robust** process, that is, a process affected minimally by external sources of variability.

As an example of an experiment, suppose that a metallurgical engineer is interested in studying the effect of two different hardening processes, oil quenching and saltwater quenching, on an aluminum alloy. Here the objective of the experimenter is to determine which quenching solution produces the maximum hardness for this particular alloy. The engineer decides to subject a number of alloy specimens or test coupons to each quenching medium and measure the hardness of the specimens after quenching. The average hardness of the specimens treated in each quenching solution will be used to determine which solution is best.

As we consider this simple experiment, a number of important questions come to mind:

1. Are these two solutions the only quenching media of potential interest?
2. Are there any other factors that might affect hardness that should be investigated or controlled in this experiment?
3. How many coupons of alloy should be tested in each quenching solution?
4. How should the test coupons be assigned to the quenching solutions, and in what order should the data be collected?

5. What method of data analysis should be used?
6. What difference in average observed hardness between the two quenching media will be considered important?

All of these questions, and perhaps many others, will have to be answered satisfactorily before the experiment is performed.

In any experiment, the results and conclusions that can be drawn depend to a large extent on the manner in which the data were collected. To illustrate this point, suppose that the metallurgical engineer in the above experiment used specimens from one heat in the oil quench and specimens from a second heat in the saltwater quench. Now, when the mean hardness is compared, the engineer is unable to say how much of the observed difference is the result of the quenching media and how much is the result of inherent differences between the heats.[1] Thus, the method of data collection has adversely affected the conclusions that can be drawn from the experiment.

In general, experiments are used to study the performance of processes and systems. The process or system can be represented by the model shown in Figure 1-1. We can usually visualize the process as a combination of machines, methods, people, and other resources that transforms some input (often a material) into an output that has one or more observable responses. Some of the process variables $x_1, x_2, \ldots, x_p$ are controllable, whereas other variables $z_1, z_2, \ldots, z_q$ are uncontrollable (although they may be controllable for purposes of a test). The objectives of the experiment may include the following:

1. Determining which variables are most influential on the response y
2. Determining where to set the influential x's so that y is almost always near the desired nominal value
3. Determining where to set the influential x's so that variability in y is small.
4. Determining where to set the influential x's so that the effects of the uncontrollable variables $z_1, z_2, \ldots, z_q$ are minimized.

As you can see from the foregoing discussion, experiments often involve several factors. Usually, an objective of the person conducting the experiment, called the **experimenter**, is to determine the influence that these factors have on the output response

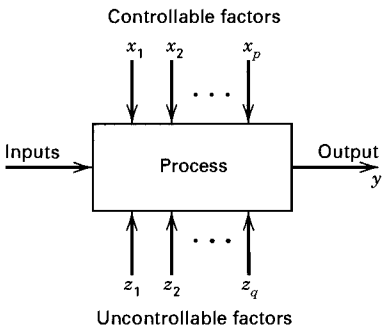


Figure 1-1 General model of a process or system.

[1] A specialist in experimental design would say that the effects of quenching media and heat were *confounded*; that is, the effects of these two factors cannot be separated.

of the system. The general approach to planning and conducting the experiment is called the **strategy of experimentation**. There are several strategies that an experimenter could use. We will illustrate some of these with a very simple example.

The author really likes to play golf. Unfortunately, he does not enjoy practicing, so he is always looking for a simpler solution to lowering his score. Some of the factors that he thinks may be important, or that may influence his golf score, are as follows:

1. The type of driver used (oversized or regular-sized)
2. The type of ball used (balata or three-piece)
3. Walking and carrying the golf clubs or riding in a golf cart
4. Drinking water or drinking beer while playing
5. Playing in the morning or playing in the afternoon
6. Playing when it is cool or playing when it is hot
7. The type of golf shoe spike worn (metal or soft)
8. Playing on a windy day or playing on a calm day

There are obviously many other factors that could be considered, but let's assume that these are the ones of primary interest. Furthermore, based on long experience with the game, he decides that factors 5 through 8 can be ignored; that is, these factors are not important because their effects are so small that they have no practical value. Engineers and scientists often must make these types of decisions about some of the factors they are considering in real experiments.

Now, let's consider how factors 1 through 4 could be experimentally tested to determine their effect on the author's golf score. Suppose that a maximum of eight rounds of golf can be played over the course of the experiment. One approach would be to select an arbitrary combination of these factors, test them, and see what happens. For example, suppose the oversized driver, balata ball, golf cart, and water combination is selected, and the resulting score is 87. During the round, however, the author noticed several wayward shots with the big driver (long is not always good in golf), and, as a result, he decides to play another round with the regular-sized driver, holding the other factors at the same levels used previously. This approach could be continued almost indefinitely, switching the levels of one (or perhaps two) factors for the next test, based on the outcome of the current test. This strategy of experimentation, which we call the **best-guess approach**, is used frequently in practice by engineers and scientists. It often works reasonably well, too, because the experimenters often have a great deal of technical or theoretical knowledge of the system they are studying, as well as considerable practical experience. There are, however, at least two disadvantages of the best-guess approach. First, suppose the initial best-guess does not produce the desired results. Now the experimenter has to take another guess at the correct combination of factor levels. This could continue for a long time, without any guarantee of success. Second, suppose the initial best-guess produces an acceptable result. Now the experimenter is tempted to stop testing, although there is no guarantee that the *best* solution has been found.

Another strategy of experimentation that is used extensively in practice is the **one-factor-at-a-time** approach. This method consists of selecting a starting point, or **baseline** set of levels, for each factor, then successively varying each factor over its range with the other factors held constant at the baseline level. After all tests are performed, a series of graphs are usually constructed showing how the response variable is affected by vary-

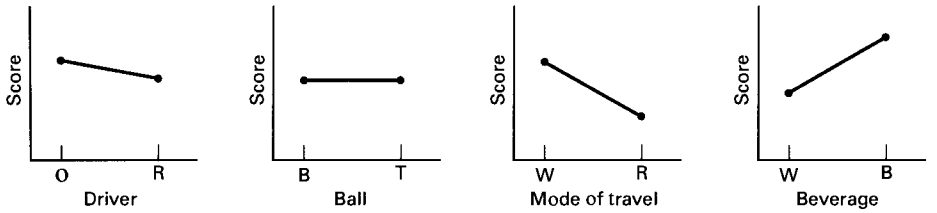


Figure 1-2 Results of the one-factor-at-a-time strategy for the golf experiment.

ing each factor with all other factors held constant. Figure 1-2 shows a set of these graphs for the golf experiment, using the oversized driver, balata ball, walking, and drinking water levels of the four factors as the baseline. The interpretation of this graph is straightforward; for example, because the slope of the mode of travel curve is negative, we would conclude that riding improves the score. Using these one-factor-at-a-time graphs, we would select the optimal combination to be the regular-sized driver, riding, and drinking water. The type of golf ball seems unimportant.

The major disadvantage of the one-factor-at-a-time strategy is that it fails to consider any possible **interaction** between the factors. An interaction is the failure of the one factor to produce the same effect on the response at different levels of another factor. Figure 1-3 shows an interaction between the type of driver and the beverage factors for the golf experiment. Notice that if the author uses the regular-sized driver, the type of beverage consumed has virtually no effect on his score, but if he uses the oversized driver, much better results are obtained by drinking water instead of beer. Interactions between factors are very common, and if they occur, the one-factor-at-a-time strategy will usually produce poor results. Many people do not recognize this, and, consequently, one-factor-at-a-time experiments are run frequently in practice. (Some individuals actually think that this strategy is related to the scientific method or that it is a "sound" engineering principle.) One-factor-at-a-time experiments are always less efficient than other methods based on a statistical approach to design. We will discuss this in more detail in Chapter 5.

The correct approach to dealing with several factors is to conduct a **factorial** experiment. This is an experimental strategy in which factors are varied *together*, instead of one at a time. The factorial experimental design concept is extremely important, and

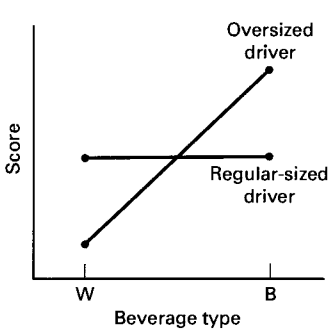


Figure 1-3 Interaction between type of driver and type of beverage for the golf experiment.

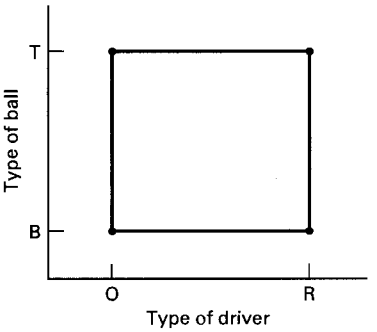


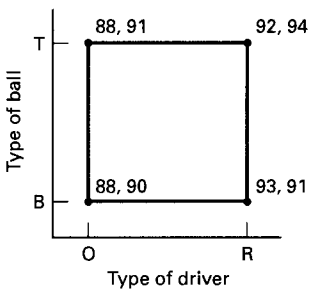
Figure 1-4 A two-factor factorial experiment involving type of driver and type of ball.

several chapters in this book are devoted to presenting basic factorial experiments and a number of useful variations and special cases.

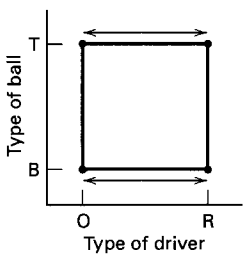
To illustrate how a factorial experiment is conducted, consider the golf experiment and suppose that only two factors, type of driver and type of ball, are of interest. Figure 1-4 shows a two-factor factorial experiment for studying the joint effects of these two factors on the author's golf score. Notice that this factorial experiment has both factors at two levels and that all possible combinations of the two factors across their levels are used in the design. Geometrically, the four runs form the corners of a square. This particular type of factorial experiment is called a $\mathbf{2^2}$ **factorial design** (two factors, each at two levels). Because the author can reasonably expect to play eight rounds of golf to investigate these factors, a reasonable plan would be to play two rounds of golf at each combination of factor levels shown in Figure 1-4. An experimental designer would say that we have **replicated** the design twice. This experimental design would enable the experimenter to investigate the individual effects of each factor (or the **main** effects) and to determine whether the factors interact.

Figure 1-5*a* shows the results of performing the factorial experiment in Figure 1-4. The scores from each round of golf played at the four test combinations are shown at the corners of the square. Notice that there are four rounds of golf that provide information about using the regular-sized driver and four rounds that provide information about using the oversized driver. By finding the average difference in the scores on the right- and left-hand sides of the square (as in Figure 1-5*b*), we have a measure of the effect of switching from the oversized driver to the regular-sized driver, or

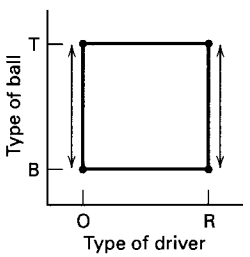
$$\text{Driver Effect} = \frac{92 + 94 + 93 + 91}{4} - \frac{88 + 91 + 88 + 90}{4}$$
$$= 3.25$$



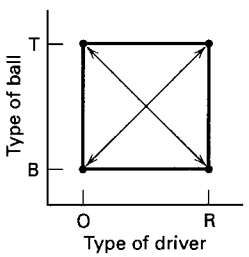
(*a*) Scores from the golf experiment



(*b*) Comparison of scores leading to the driver effect



(*c*) Comparison of scores leading to the ball effect



(*d*) Comparison of scores leading to the ball-driver interaction effect

Figure 1-5 Scores from the golf experiment in Figure 1-4 and calculation of the factor effects.

That is, on average, switching from the oversized to the regular-sized driver increases the score by 3.25 strokes per round. Similarly, the average difference in the four scores at the top of the square and the four scores at the bottom measure the effect of the type of ball used (see Figure 1-5*c*):

$$\text{Ball Effect} = \frac{88 + 91 + 92 + 94}{4} - \frac{88 + 90 + 93 + 91}{4}$$
$$= 0.75$$

Finally, a measure of the interaction effect between the type of ball and the type of driver can be obtained by subtracting the average scores on the left-to-right diagonal in the square from the average scores on the right-to-left diagonal (see Figure 1-5*d*), resulting in

$$\text{Ball–Driver Interaction Effect} = \frac{92 + 94 + 88 + 90}{4} - \frac{88 + 91 + 93 + 91}{4}$$
$$= 0.25$$

The results of this factorial experiment indicate that driver effect is larger than either the ball effect or the interaction. Statistical testing could be used to determine whether any of these effects differ from zero. In fact, it turns out that there is reasonably strong statistical evidence that the driver effect differs from zero and the other two effects do not. Therefore, perhaps the author should always play with the oversized driver.

One very important feature of the factorial experiment is evident from this simple example; namely, factorials make the most efficient use of the experimental data. Notice that this experiment included eight observations, and all eight observations are used to calculate the driver, the ball, and interaction effects. No other strategy of experimentation makes so efficient use of the data. This is an important and useful feature of factorials.

We can extend the factorial experiment concept to three factors. Suppose that the author wishes to study the effects of type of driver, type of ball, and the type of beverage consumed on his golf score. Assuming that all three factors have two levels, a factorial design can be set up as shown in Figure 1-6. Notice that there are eight test combinations of these three factors across the two levels of each and that these eight trials can be represented geometrically as the corners of a cube. This is an example of a **2^3 factorial design**. Because the author only wants to play eight rounds of golf, this experiment would require that one round be played at each combination of factors represented by the eight corners of the cube in Figure 1-6. However, if we compare this to the two-factor factorial in Figure 1-4, the 2^3 factorial design would provide the same information about the factor

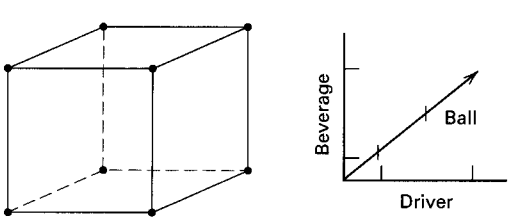


Figure 1-6 A three-factor factorial experiment involving type of driver, type of ball, and type of beverage.

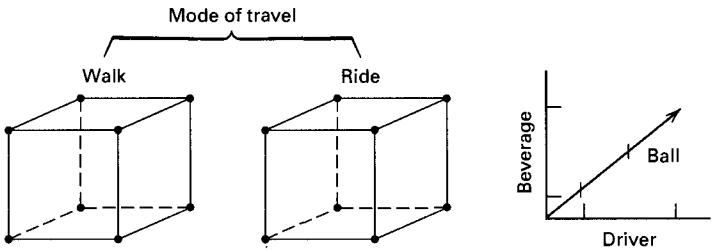


Figure 1-7 A four-factor factorial experiment involving type of driver, type of ball, type of beverage, and mode of travel.

effects. For example, in both designs there are four tests that provide information about the regular-sized driver and four tests that provide information about the oversized driver, assuming that each run in the two-factor design in Figure 1-4 is replicated twice.

Figure 1-7 illustrates how all four factors—driver, ball, beverage, and mode of travel (walking or riding)—could be investigated in a 2^4 **factorial design**. As in any factorial design, all possible combinations of the levels of the factors are used. Because all four factors are at two levels, this experimental design can still be represented geometrically as a cube (actually a hypercube).

Generally, if there are k factors, each at two levels, the factorial design would require 2^k runs. For example, the experiment in Figure 1-7 requires 16 runs. Clearly, as the number of factors of interest increases, the number of runs required increases rapidly; for instance, a 10-factor experiment with all factors at two levels would require 1024 runs. This quickly becomes infeasible from a time and resource viewpoint. In the golf experiment, the author can only play eight rounds of golf, so even the experiment in Figure 1-7 is too large.

Fortunately, if there are four to five or more factors, it is usually unnecessary to run all possible combinations of factor levels. A **fractional factorial experiment** is a variation of the basic factorial design in which only a subset of the runs are made. Figure 1-8 shows a fractional factorial design for the four-factor version of the golf experiment. This design requires only 8 runs instead of the original 16 and would be called a **one-half fraction**. If the author can only play eight rounds of golf, this is an excellent design in which to study all four factors. It will provide good information about the main effects of the four factors as well as some information about how these factors interact.

Fractional factorial designs are used extensively in industrial research and development, and for process improvement. These designs will be discussed in Chapter 8.

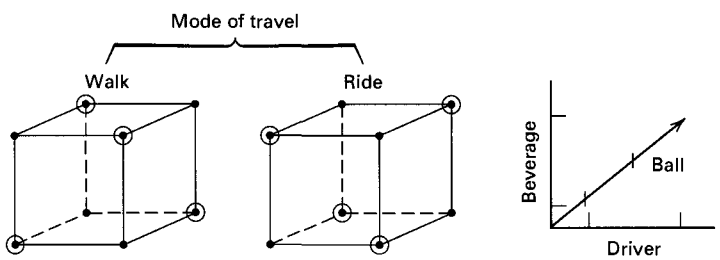


Figure 1-8 A four-factor fractional factorial experiment involving type of driver, type of ball, type of beverage, and mode of travel.

1-2 SOME TYPICAL APPLICATIONS OF EXPERIMENTAL DESIGN

Experimental design methods have found broad application in many disciplines. In fact, we may view experimentation as part of the scientific process and as one of the ways we learn about how systems or processes work. Generally, we learn through a series of activities in which we make conjectures about a process, perform experiments to generate data from the process, and then use the information from the experiment to establish new conjectures, which lead to new experiments, and so on.

Experimental design is a critically important tool in the engineering world for improving the performance of a manufacturing process. It also has extensive application in the development of new processes. The application of experimental design techniques early in process development can result in

1. Improved process yields
2. Reduced variability and closer conformance to nominal or target requirements
3. Reduced development time
4. Reduced overall costs

Experimental design methods also play a major role in **engineering design** activities, where new products are developed and existing ones improved. Some applications of experimental design in engineering design include

1. Evaluation and comparison of basic design configurations
2. Evaluation of material alternatives
3. Selection of design parameters so that the product will work well under a wide variety of field conditions, that is, so that the product is **robust**
4. Determination of key product design parameters that impact product performance

The use of experimental design in these areas can result in products that are easier to manufacture, products that have enhanced field performance and reliability, lower product cost, and shorter product design and development time. We now present several examples that illustrate some of these ideas.

EXAMPLE 1-1

Characterizing a Process

A flow solder machine is used in the manufacturing process for printed circuit boards. The machine cleans the boards in a flux, preheats the boards, and then moves them along a conveyor through a wave of molten solder. This solder process makes the electrical and mechanical connections for the leaded components on the board.

The process currently operates around the 1 percent defective level. That is, about 1 percent of the solder joints on a board are defective and require manual retouching. However, because the average printed circuit board contains over 2000 solder joints, even a 1 percent defective level results in far too many solder joints requiring rework. The process engineer responsible for this area would like to use a designed experiment to determine which machine parameters are influential in the occurrence of solder defects and which adjustments should be made to those variables to reduce solder defects.

The flow solder machine has several variables that can be controlled. They include

1. Solder temperature
2. Preheat temperature
3. Conveyor speed
4. Flux type
5. Flux specific gravity
6. Solder wave depth
7. Conveyor angle

In addition to these controllable factors, there are several other factors that cannot be easily controlled during routine manufacturing, although they could be controlled for the purposes of a test. They are

1. Thickness of the printed circuit board
2. Types of components used on the board
3. Layout of the components on the board
4. Operator
5. Production rate

In this situation, the engineer is interested in **characterizing** the flow solder machine; that is, he wants to determine which factors (both controllable and uncontrollable) affect the occurrence of defects on the printed circuit boards. To accomplish this, he can design an experiment that will enable him to estimate the magnitude and direction of the factor effects; that is, how much does the response variable (defects per unit) change when each factor is changed, and does changing the factors *together* produce different results than are obtained from individual factor adjustments—that is, do the factors interact? Sometimes we call an experiment such as this a **screening experiment**. Typically, screening or characterization experiments involve using fractional factorial designs, such as in the golf example in Figure 1-8.

The information from this screening or characterization experiment will be used to identify the critical process factors and to determine the direction of adjustment for these factors to reduce further the number of defects per unit. The experiment may also provide information about which factors should be more carefully controlled during routine manufacturing to prevent high defect levels and erratic process performance. Thus, one result of the experiment could be the application of techniques such as control charts to one or more **process variables** (such as solder temperature), in addition to control charts on process output. Over time, if the process is improved enough, it may be possible to base most of the process control plan on controlling process input variables instead of control charting the output.

EXAMPLE 1-2

Optimizing a Process

In a characterization experiment, we are usually interested in determining which process variables affect the response. A logical next step is to optimize, that is, to determine the

region in the important factors that leads to the best possible response. For example, if the response is yield, we would look for a region of maximum yield, whereas if the response is variability in a critical product dimension, we would seek a region of minimum variability.

Suppose that we are interested in improving the yield of a chemical process. We know from the results of a characterization experiment that the two most important process variables that influence the yield are operating temperature and reaction time. The process currently runs at 145°F and 2.1 hours of reaction time, producing yields of around 80 percent. Figure 1-9 shows a view of the time–temperature region from above. In this graph, the lines of constant yield are connected to form response **contours**, and we have shown the contour lines for yields of 60, 70, 80, 90, and 95 percent. These contours are projections on the time–temperature region of cross sections of the yield surface corresponding to the aforementioned percent yields. This surface is sometimes called a **response surface**. The true response surface in Figure 1-9 is unknown to the process personnel, so experimental methods will be required to optimize the yield with respect to time and temperature.

To locate the optimum, it is necessary to perform an experiment that varies time and temperature together, that is, a factorial experiment. The results of an initial factorial experiment with both time and temperature run at two levels is shown in Figure 1-9. The responses observed at the four corners of the square indicate that we should move in the general direction of increased temperature and decreased reaction time to increase yield.

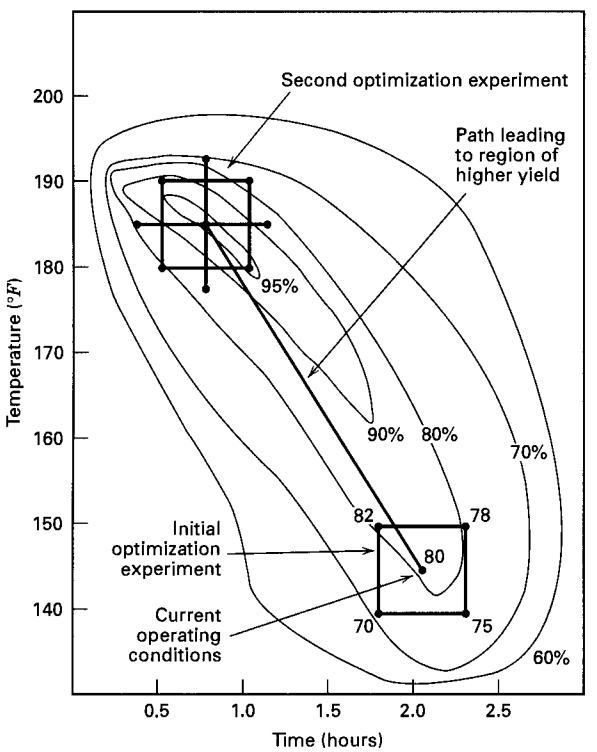


Figure 1-9 Contour plot of yield as a function of reaction time and reaction temperature, illustrating experimentation to optimize a process.

A few additional runs would be performed in this direction, and this additional experimentation would lead us to the region of maximum yield.

Once we have found the region of the optimum, a second experiment would typically be performed. The objective of this second experiment is to develop an empirical model of the process and to obtain a more precise estimate of the optimum operating conditions for time and temperature. This approach to process optimization is called **response surface methodology**, and it is explored in detail in Chapter 11. The second design illustrated in Figure 1-9 is a **central composite design**, one of the most important experimental designs used in process optimization studies.

EXAMPLE 1-3

A Product Design Example

Experimental design methods can often be applied to the product design process. To illustrate, suppose that a group of engineers is designing a door hinge for an automobile. The quality characteristic of interest is the check effort, or the holding ability of the door latch that prevents the door from swinging closed when the vehicle is parked on a hill. The check mechanism consists of a leaf spring and a roller. When the door is opened, the roller travels through an arc, causing the leaf spring to be compressed. To close the door, the spring must be forced aside, and this creates the check effort. The engineering team thinks that check effort is a function of the following factors:

1. Roller travel distance
2. Spring height from pivot to base
3. Horizontal distance from pivot to spring
4. Free height of the reinforcement spring
5. Free height of the main spring

The engineers can build a prototype hinge mechanism in which all of these factors can be varied over certain ranges. Once appropriate levels for these five factors have been identified, an experiment can be designed consisting of various combinations of the factor levels, and the prototype hinge can be tested at these combinations. This will produce information concerning which factors are most influential on the latch check effort, and through analysis of this information, the latch design can be improved.

1-3 BASIC PRINCIPLES

If an experiment such as the ones described in Examples 1-1 through 1-3 is to be performed most efficiently, a scientific approach to planning the experiment must be employed. **Statistical design of experiments** refers to the process of planning the experiment so that appropriate data that can be analyzed by statistical methods will be collected, resulting in valid and objective conclusions. The statistical approach to experimental design is necessary if we wish to draw meaningful conclusions from the data. When the problem involves data that are subject to experimental errors, statistical methodology is the only objective approach to analysis. Thus, there are two aspects to any experimental problem: the design of the experiment and the statistical analysis of the

data. These two subjects are closely related because the method of analysis depends directly on the design employed. Both topics will be addressed in this book.

The three basic principles of experimental design are **replication**, **randomization**, and **blocking**. By replication we mean a repetition of the basic experiment. In the metallurgical experiment discussed in Section 1-1, replication would consist of treating a specimen by oil quenching and treating a specimen by saltwater quenching. Thus, if five specimens are treated in each quenching medium, we say that five **replicates** have been obtained. Replication has two important properties. First, it allows the experimenter to obtain an estimate of the experimental error. This estimate of error becomes a basic unit of measurement for determining whether observed differences in the data are really *statistically* different. Second, if the sample mean (e.g., $\bar{y}$) is used to estimate the effect of a factor in the experiment, replication permits the experimenter to obtain a more precise estimate of this effect. For example; if σ^2 is the variance of an individual observation and there are n replicates, the variance of the sample mean is

$$\sigma_{\bar{y}}^2 = \frac{\sigma^2}{n}$$

The practical implication of this is that if we had $n = 1$ replicates and observed $y_1 = 145$ (oil quench) and $y_2 = 147$ (saltwater quench), we would probably be unable to make satisfactory inferences about the effect of the quenching medium—that is, the observed difference could be the result of experimental error. On the other hand, if n was reasonably large, and the experimental error was sufficiently small and if we observed $\bar{y}_1 < \bar{y}_2$, we would be reasonably safe in concluding that saltwater quenching produces a higher hardness in this particular aluminum alloy than does oil quenching.

There is an important distinction between replication and **repeated measurements**. For example, suppose that a silicon wafer is etched in a single-wafer plasma etching process, and a critical dimension on this wafer is measured three times. These measurements are not replicates; they are a form of repeated measurements, and in this case, the observed variability in the three repeated measurements is a direct reflection of the inherent variability in the measurement system or gauge. As another illustration, suppose that as part of an experiment in semiconductor manufacturing, four wafers are processed simultaneously in an oxidation furnace at a particular gas flow rate and time and then a measurement is taken on the oxide thickness of each wafer. Once again, the measurement on the four wafers are not replicates but repeated measurements. In this case they reflect differences among the wafers and other sources of variability within that particular furnace run. Replication reflects sources of variability both **between** runs and (potentially) **within** runs.

Randomization is the cornerstone underlying the use of statistical methods in experimental design. By randomization we mean that both the allocation of the experimental material and the order in which the individual runs or trials of the experiment are to be performed are randomly determined. Statistical methods require that the observations (or errors) be independently distributed random variables. Randomization usually makes this assumption valid. By properly randomizing the experiment, we also assist in "averaging out" the effects of extraneous factors that may be present. For example, suppose that the specimens in the above experiment are of slightly different thicknesses and that the effectiveness of the quenching medium may be affected by specimen thickness. If all the specimens subjected to the oil quench are thicker than those subjected to the saltwater quench, we may be introducing systematic bias into the experimental results.

This bias handicaps one of the quenching media and consequently invalidates our results. Randomly assigning the specimens to the quenching media alleviates this problem.

Computer software programs are widely used to assist experimenters in selecting and constructing experimental designs. These programs often present the runs in the experimental design in random order. This random order is usually created by using a random number generator. Even with such a computer program, it is still often necessary to assign experimental material (such as the wafers in the semiconductor examples mentioned above), operators, gauges or measurement devices, and so forth, for use in the experiment. Tables of random numbers can be used to ensure that random assignments are made.

Sometimes experimenters encounter situations where randomization of some aspect of the experiment is difficult. For example, in a chemical process, temperature may be a very hard-to-change variable, making **complete randomization** of this factor almost impossible. There are statistical design methods for dealing with restrictions on randomization. Some of these approaches will be discussed in subsequent chapters (see in particular, Chapter 13).

Blocking is a design technique used to improve the precision with which comparisons among the factors of interest are made. Often blocking is used to reduce or eliminate the variability transmitted from **nuisance factors**; that is, factors that may influence the experimental response but in which we are not directly interested. For example, an experiment in a chemical process may require two batches of raw material to make all the required runs. However, there could be differences between the batches due to supplier-to-supplier variability, and if we are not specifically interested in this effect, we would think of the batches of raw material as a nuisance factor. Generally, a block is a set of relatively homogeneous experimental conditions. In the chemical process example, each batch of raw material would form a block, because the variability within a batch would be expected to be smaller than the variability between batches. Typically, as in this example, each level of the nuisance factor becomes a block. Then the experimenter divides the observations from the statistical design into groups that are run in each block. We study blocking in detail in several places in the text, including Chapters 4, 5, 7, 8, 9, 11, and 13. A simple example illustrating the blocking principal is given in Chapter 2, Section 2-5.1.

The three basic principles of experimental design, randomization, replication, and blocking are part of every experiment. We will illustrate and emphasize them repeatedly throughout this book.

1-4 GUIDELINES FOR DESIGNING EXPERIMENTS

To use the statistical approach in designing and analyzing an experiment, it is necessary for everyone involved in the experiment to have a clear idea in advance of exactly what is to be studied, how the data are to be collected, and at least a qualitative understanding of how these data are to be analyzed. An outline of the recommended procedure is shown in Table 1-1 on the next page. We now give a brief discussion of this outline and elaborate on some of the key points. For more details, see Coleman and Montgomery (1993), and the references therein. The supplemental text material for this chapter is also useful.

*1. **Recognition of and statement of the problem.*** This may seem to be a rather obvious point, but in practice it is often not simple to realize that a problem requiring experi-

Table 1-1 Guidelines for Designing an Experiment

1. Recognition of and statement of the problem.	Pre-experimental planning
2. Choice of factors, levels, and ranges.[a]	
3. Selection of the response variable.[a]	
4. Choice of experimental design.	
5. Performing the experiment.	
6. Statistical analysis of the data.	
7. Conclusions and recommendations.	

[a] In practice, steps 2 and 3 are often done simultaneously or in reverse order.

mentation exists, nor is it simple to develop a clear and generally accepted statement of this problem. It is necessary to develop all ideas about the objectives of the experiment. Usually, it is important to solicit input from all concerned parties: engineering, quality assurance, manufacturing, marketing, management, the customer, and operating personnel (who usually have much insight and who are too often ignored). For this reason a **team approach** to designing experiments is recommended.

It is usually helpful to prepare a list of specific problems or questions that are to be addressed by the experiment. A clear statement of the problem often contributes substantially to better understanding of the phenomenon being studied and the final solution of the problem. It is also important to keep the overall objective in mind; for example, is this a new process or system—in which case the initial objective is likely to be characterization or factor screening—or is it a mature or reasonably well-understood system that has been previously characterized—in which case the objective may be optimization? There are many possible objectives of an experiment, including confirmation (is the system performing the same way now that it did in the past?), discovery (what happens if we explore new materials, variables, operating conditions, etc.?), and stability (under what conditions do the response variables of interest seriously degrade?). Obviously, the specific questions to be addressed in the experiment relate directly to the overall objectives. Often at this stage of problem formulation many engineers and scientists realize that one large **comprehensive** experiment is unlikely to answer the key questions and that a **sequential approach** using a series of smaller experiments is a better strategy.

2. Choice of factors, levels, and range. (As noted in Table 1-1, steps 2 and 3 are often done simultaneously, or in the reverse order.) When considering the factors that may influence the performance of a process or system, the experimenter usually discovers that these factors can be classified as either **potential design factors** or nuisance factors. The potential design factors are those factors that the experimenter may wish to vary in the experiment. Often we find that there are a lot of potential design factors, and some further classification of them is helpful. Some useful classifications are **design factors**, **held-constant factors**, and **allowed-to-vary** factors. The design factors are the factors actually selected for study in the experiment. Held-constant factors are variables that may exert some effect on the response, but for purposes of the present experiment these factors are not of interest, so they will be held at a specific level. For example, in an etching experiment in the semiconductor industry there may be an effect that is unique to the specific plasma etch tool used in the experiment. However, this factor would be very difficult to vary in an experiment, so the experimenter may decide to perform all experimental runs on one particular (ideally "typical") etcher. Thus this factor has been held constant. As an example of allowed-to-vary factors, the experimental units or the "materials" to which the design factors are applied are usually nonhomogeneous, yet we

often ignore this unit-to-unit variability and rely on randomization to balance out any material or experimental unit effect. We often assume that the effects of held-constant factors and allowed-to-vary factors are relatively small.

Nuisance factors, on the other hand, may have large effects that must be accounted for, yet we may not be interested in them in the context of the present experiment. Nuisance factors are often classified as **controllable, uncontrollable,** or **noise factors.** A controllable nuisance factor is one whose levels may be set by the experimenter. For example, the experimenter can select different batches of raw material or different days of the week when conducting the experiment. The blocking principal, discussed in the previous section, is often useful in dealing with controllable nuisance factors. If a nuisance factor is uncontrollable in the experiment, but it can be measured, an analysis procedure called the **analysis of covariance** can often be used to compensate for its effect. For example, the relative humidity in the process environment may affect process performance, and if the humidity cannot be controlled, it probably can be measured and treated as a covariate. When a factor that varies naturally and uncontrollably in the process can be controlled for purposes of an experiment, we often call it a noise factor. In such situations, our objective is usually to find the settings of the controllable design factors that minimize the variability transmitted from the noise factors. This is sometimes called a process robustness study or a robust design problem. Blocking, analysis of covariance, and process robustness studies are discussed later in the text.

Once the experimenter has selected the design factors, he or she must choose the ranges over which these factors will be varied, and the specific levels at which runs will be made. Thought must also be given to how these factors are to be controlled at the desired values and how they are to be measured. For instance, in the flow solder experiment, the engineer has defined 12 variables that may affect the occurrence of solder defects. The engineer will also have to decide on a region of interest for each variable (that is, the range over which each factor will be varied) and on how many levels of each variable to use. **Process knowledge** is required to do this. This process knowledge is usually a combination of practical experience and theoretical understanding. It is important to investigate all factors that may be of importance and to not be overly influenced by past experience, particularly when we are in the early stages of experimentation or when the process is not very mature.

When the objective of the experiment is factor screening or process characterization, it is usually best to keep the number of factor levels low. Generally, two levels work very well in factor screening studies. Choosing the region of interest is also important. In factor screening, the region of interest should be relatively large—that is, the range over which the factors are varied should be broad. As we learn more about which variables are important and which levels produce the best results, the region of interest will usually become narrower.

*3. **Selection of the response variable.*** In selecting the response variable, the experimenter should be certain that this variable really provides useful information about the process under study. Most often, the average or standard deviation (or both) of the measured characteristic will be the response variable. Multiple responses are not unusual. Gauge capability (or measurement error) is also an important factor. If gauge capability is inadequate, only relatively large factor effects will be detected by the experiment or perhaps additional replication will be required. In some situations where gauge capability is poor, the experimenter may decide to measure each experimental unit several times

and use the average of the repeated measurements as the observed response. It is usually critically important to identify issues related to defining the responses of interest and how they are to be measured *before* conducting the experiment. Sometimes designed experiments are employed to study and improve the performance of measurement systems. For an example, see Chapter 12.

We reiterate how crucial it is to bring out all points of view and process information in steps 1 through 3 above. We refer to this as **pre-experimental planning**. Coleman and Montgomery (1993) provide worksheets that can be useful in pre-experimental planning. Also see the supplemental text information for more details and an example of using these worksheets. It is unlikely that one person has all the knowledge required to do this adequately in many situations. Therefore, we argue strongly for a team effort in planning the experiment. Most of your success will hinge on how well the pre-experimental planning is done.

4. Choice of experimental design. If the pre-experimental planning activities above are done correctly, this step is relatively easy. Choice of design involves the consideration of sample size (number of replicates), the selection of a suitable run order for the experimental trials, and the determination of whether or not blocking or other randomization restrictions are involved. This book discusses some of the more important types of experimental designs, and it can ultimately be used as a catalog for selecting an appropriate experimental design for a wide variety of problems.

There are also several interactive statistical software packages that support this phase of experimental design. The experimenter can enter information about the number of factors, levels, and ranges, and these programs will either present a selection of designs for consideration or recommend a particular design. (We prefer to see several alternatives instead of relying on a computer recommendation in most cases.) These programs will usually also provide a worksheet (with the order of the runs randomized) for use in conducting the experiment.

In selecting the design, it is important to keep the experimental objectives in mind. In many engineering experiments, we already know at the outset that some of the factor levels will result in different values for the response. Consequently, we are interested in identifying *which* factors cause this difference and in estimating the *magnitude* of the response change. In other situations, we may be more interested in verifying uniformity. For example, two production conditions A and B may be compared, A being the standard and B being a more cost-effective alternative. The experimenter will then be interested in demonstrating that, say, there is no difference in yield between the two conditions.

5. Performing the experiment. When running the experiment, it is vital to monitor the process carefully to ensure that everything is being done according to plan. Errors in experimental procedure at this stage will usually destroy experimental validity. Up-front planning is crucial to success. It is easy to underestimate the logistical and planning aspects of running a designed experiment in a complex manufacturing or research and development environment.

Coleman and Montgomery (1993) suggest that prior to conducting the experiment a few trial runs or pilot runs are often helpful. These runs provide information about consistency of experimental material, a check on the measurement system, a rough idea of experimental error, and a chance to practice the overall experimental technique. This also provides an opportunity to revisit the decisions made in steps 1–4, if necessary.

6. Statistical analysis of the data. Statistical methods should be used to analyze the data so that results and conclusions are *objective* rather than judgmental in nature. If the experiment has been designed correctly and if it has been performed according to the design, the statistical methods required are not elaborate. There are many excellent software packages designed to assist in data analysis, and many of the programs used in step 4 to select the design provide a seamless, direct interface to the statistical analysis. Often we find that simple graphical methods play an important role in data analysis and interpretation. Because many of the questions that the experimenter wants to answer can be cast into an hypothesis-testing framework, hypothesis testing and confidence interval estimation procedures are very useful in analyzing data from a designed experiment. It is also usually very helpful to present the results of many experiments in terms of an **empirical model**, that is, an equation derived from the data that expresses the relationship between the response and the important design factors. Residual analysis and model adequacy checking are also important analysis techniques. We will discuss these issues in detail later.

Remember that statistical methods cannot prove that a factor (or factors) has a particular effect. They only provide guidelines as to the reliability and validity of results. Properly applied, statistical methods do not allow anything to be proved experimentally, but they do allow us to measure the likely error in a conclusion or to attach a level of confidence to a statement. The primary advantage of statistical methods is that they add objectivity to the decision-making process. Statistical techniques coupled with good engineering or process knowledge and common sense will usually lead to sound conclusions.

7. Conclusions and recommendations. Once the data have been analyzed, the experimenter must draw *practical* conclusions about the results and recommend a course of action. Graphical methods are often useful in this stage, particularly in presenting the results to others. **Follow-up runs** and **confirmation testing** should also be performed to validate the conclusions from the experiment.

Throughout this entire process, it is important to keep in mind that experimentation is an important part of the learning process, where we tentatively formulate hypotheses about a system, perform experiments to investigate these hypotheses, and on the basis of the results formulate new hypotheses, and so on. This suggests that experimentation is **iterative**. It is usually a major mistake to design a single, large, comprehensive experiment at the start of a study. A successful experiment requires knowledge of the important factors, the ranges over which these factors should be varied, the appropriate number of levels to use, and the proper units of measurement for these variables. Generally, we do not perfectly know the answers to these questions, but we learn about them as we go along. As an experimental program progresses, we often drop some input variables, add others, change the region of exploration for some factors, or add new response variables. Consequently, we usually experiment *sequentially*, and as a general rule, no more than about 25 percent of the available resources should be invested in the first experiment. This will ensure that sufficient resources are available to perform confirmation runs and ultimately accomplish the final objective of the experiment.

1-5 A BRIEF HISTORY OF STATISTICAL DESIGN

There have been four eras in the modern development of statistical experimental design. The agricultural era was led by the pioneering work of Sir Ronald A. Fisher in the 1920s

and early 1930s. During this time, Fisher was responsible for statistics and data analysis at the Rothamsted Agricultural Experimental Station near London, England. Fisher recognized that flaws in the way the experiment that generated the data had been performed often hampered the analysis of data from systems (in this case agricultural systems). By interacting with scientists and researchers in many fields he developed the insights that led to the three basic principles of experimental design that we discussed in Section 1-3: randomization, replication, and blocking. Fisher systematically introduced statistical thinking and principles into designing experimental investigations, including the factorial design concept and the analysis of variance. His two books [Fisher (1958, 1966)] had profound influence on the use of statistics, particularly in agricultural and related life sciences. For an excellent biography of Fisher, see Box (1978).

Although applications of statistical design in industrial settings certainly began in the 1930s, the second, or industrial, era was catalyzed by the development of response surface methodology (RSM) by Box and Wilson (1951). They recognized and exploited the fact that many industrial experiments are fundamentally different from their agricultural counterparts in two ways: (1) the response variable can usually be observed (nearly) immediately, and (2) the experimenter can quickly learn crucial information from a small group of runs that can be used to plan the next experiment. Box (1999) calls these two features of industrial experiments *immediacy* and *sequentiality*. Over the next 30 years, RSM and other design techniques spread throughout the chemical and the process industries, mostly in research and development work. George Box was the intellectual leader of this movement. However, the application of statistical design at the plant or manufacturing process level was still not extremely widespread. Some of the reasons for this include inadequate training in basic statistical concepts and methods for engineers and other process specialists and the lack of computing resources and user-friendly statistical software to support the application of statistically designed experiments.

The increasing interest of Western industry in quality improvement that began in the late 1970s ushered in the third era of statistical design. The work of Genichi Taguchi [Taguchi and Wu (1980), Kackar (1985), and Taguchi (1987, 1991)] had a significant impact on expanding the interest in and use of designed experiments. Taguchi advocated using designed experiments for what he termed robust parameter design, or

1. Making processes insensitive to environmental factors or other factors that are difficult to control
2. Making products insensitive to variation transmitted from components
3. Finding levels of the process variables that force the mean to a desired value while simultaneously reducing variability around this value

Taguchi suggested highly fractionated factorial designs and other orthogonal arrays along with some novel statistical methods to solve these problems. The resulting methodology generated much discussion and controversy. Part of the controversy arose because Taguchi's methodology was advocated in the West initially (and primarily) by entrepreneurs, and the underlying statistical science had not been adequately peer-reviewed. By the late 1980s the results of peer review indicated that although Taguchi's engineering concepts and objectives were well-founded, there were substantial problems with his experimental strategy and methods of data analysis. For specific details of these issues, see Box (1988), Box, Bisgaard, and Fung (1988), Hunter (1985, 1989), Myers and Montgomery (1995), and Pignatiello and Ramberg (1992). Many of these concerns are also summarized in

the extensive panel discussion in the May 1992 issue of *Technometrics* [see Nair et al. (1992)].

There were at least three positive outcomes of the Taguchi controversy. First, designed experiments became more widely used in the discrete parts industries, including automotive and aerospace manufacturing, electronics and semiconductors, and many other industries that had previously made little use of the technique. Second, the fourth era of statistical design began. This era has included a renewed general interest in statistical design by both researchers and practitioners and the development of many new and useful approaches to experimental problems in the industrial world, including alternatives to Taguchi's technical methods that allow his engineering concepts to be carried into practice efficiently and effectively. Some of these alternatives will be discussed and illustrated in subsequent chapters, particularly Chapter 11. Third, formal education in statistical experimental design is becoming part of many engineering programs in universities, at both undergraduate and graduate levels. The successful integration of good experimental design practice into engineering and science is a key factor in future industrial competitiveness.

1-6 SUMMARY: USING STATISTICAL TECHNIQUES IN EXPERIMENTATION

Much of the research in engineering, science, and industry is empirical and makes extensive use of experimentation. Statistical methods can greatly increase the efficiency of these experiments and often strengthen the conclusions so obtained. The proper use of statistical techniques in experimentation requires that the experimenter keep the following points in mind:

1. Use your nonstatistical knowledge of the problem. Experimenters are usually highly knowledgeable in their fields. For example, a civil engineer working on a problem in hydrology typically has considerable practical experience and formal academic training in this area. In some fields there is a large body of physical theory on which to draw in explaining relationships between factors and responses. This type of nonstatistical knowledge is invaluable in choosing factors, determining factor levels, deciding how many replicates to run, interpreting the results of the analysis, and so forth. Using statistics is no substitute for thinking about the problem.

2. Keep the design and analysis as simple as possible. Don't be overzealous in the use of complex, sophisticated statistical techniques. Relatively simple design and analysis methods are almost always best. This is a good place to reemphasize step 4 of the procedure recommended in Section 1-4. If you do the design carefully and correctly, the analysis will almost always be relatively straightforward. However, if you botch the design badly, it is unlikely that even the most complex and elegant statistics can save the situation.

3. Recognize the difference between practical and statistical significance. Just because two experimental conditions produce mean responses that are statistically different, there is no assurance that this difference is large enough to have any practical value. For example, an engineer may determine that a modification to an automobile fuel injection

system may produce a true mean improvement in gasoline mileage of 0.1 mi/gal. This is a statistically significant result. However, if the cost of the modification is $1000, the 0.1 mi/gal difference is probably too small to be of any practical value.

4. Experiments are usually iterative. Remember that in most situations it is unwise to design too comprehensive an experiment at the start of a study. Successful design requires knowledge of the important factors, the ranges over which these factors are varied, the appropriate number of levels for each factor, and the proper methods and units of measurement for each factor and response. Generally, we are not well-equipped to answer these questions at the beginning of the experiment, but we learn the answers as we go along. This argues in favor of the *iterative*, or *sequential*, approach discussed previously. Of course, there are situations where comprehensive experiments are entirely appropriate, but as a general rule, most experiments should be iterative. Consequently, we usually should not invest more than about 25 percent of the resources of experimentation (runs, budget, time, etc.) in the initial experiment. Often these first efforts are just learning experiences, and some resources must be available to accomplish the final objectives of the experiment.

2 Simple Comparative Experiments

In this chapter, we consider experiments to compare two **conditions** (sometimes called **treatments**). These are often called **simple comparative experiments**. We begin with an example of an experiment performed to determine whether two different formulations of a product give equivalent results. The discussion leads to a review of several basic statistical concepts, such as random variables, probability distributions, random samples, sampling distributions, and tests of hypotheses.

2-1 INTRODUCTION

The tension bond strength of portland cement mortar is an important characteristic of the product. An engineer is interested in comparing the strength of a modified formulation in which polymer latex emulsions have been added during mixing to the strength of the unmodified mortar. The experimenter has collected 10 observations on strength for the modified formulation and another 10 observations for the unmodified formulation. The data are shown in Table 2-1 on the next page. We could refer to the two different formulations as two **treatments** or as two **levels** of the **factor** formulations.

The data from this experiment are plotted in Figure 2-1 on the next page. This display is called a **dot diagram**. Visual examination of these data give the immediate impression that the strength of the unmodified mortar is greater than the strength of the modified mortar. This impression is supported by comparing the *average* tension bond strengths, $\bar{y}_1 = 16.76$ kgf/cm^2 for the modified mortar and $\bar{y}_2 = 17.92$ kgf/cm^2 for the unmodified mortar. The average tension bond strengths in these two samples differ by what seems to be a nontrivial amount. However, it is not obvious that this difference is large enough to imply that the two formulations really *are* different. Perhaps this observed difference in average strengths is the result of sampling fluctuation and the two formulations are really identical. Possibly another two samples would give opposite results, with the strength of the modified mortar exceeding that of the unmodified formulation.

A technique of statistical inference called **hypothesis testing** (some prefer **significance testing**) can be used to assist the experimenter in comparing these two formula-

Table 2-1 Tension Bond Strength Data for the Portland Cement Formulation Experiment

j	Modified Mortar y_{1j}	Unmodified Mortar y_{2j}
1	16.85	17.50
2	16.40	17.63
3	17.21	18.25
4	16.35	18.00
5	16.52	17.86
6	17.04	17.75
7	16.96	18.22
8	17.15	17.90
9	16.59	17.96
10	16.57	18.15

tions. Hypothesis testing allows the comparison of the two formulations to be made on *objective* terms, with a knowledge of the risks associated with reaching the wrong conclusion. Before presenting procedures for hypothesis testing in simple comparative experiments, we will briefly summarize some elementary statistical concepts.

2-2 BASIC STATISTICAL CONCEPTS

Each of the observations in the portland cement experiment described above would be called a **run**. Notice that the individual runs differ, so there is fluctuation, or **noise**, in the results. This noise is usually called **experimental error** or simply **error**. It is a **statistical error**, meaning that it arises from variation that is uncontrolled and generally unavoidable. The presence of error or noise implies that the response variable, tension bond strength, is a **random variable**. A random variable may be either **discrete** or **continuous**. If the set of all possible values of the random variable is either finite or countably infinite, then the random variable is discrete, whereas if the set of all possible values of the random variable is an interval, then the random variable is continuous.

Graphical Description of Variability

We often use simple graphical methods to assist in analyzing the data from an experiment. The **dot diagram**, illustrated in Figure 2-1, is a very useful device for displaying a small body of data (say up to about 20 observations). The dot diagram enables the experimenter to see quickly the general **location** or **central tendency** of the observations and their **spread**. For example, in the portland cement tension bond experiment, the dot diagram

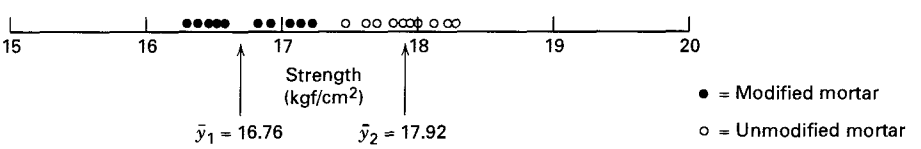


Figure 2-1 Dot diagram for the tension bond strength data in Table 2-1.

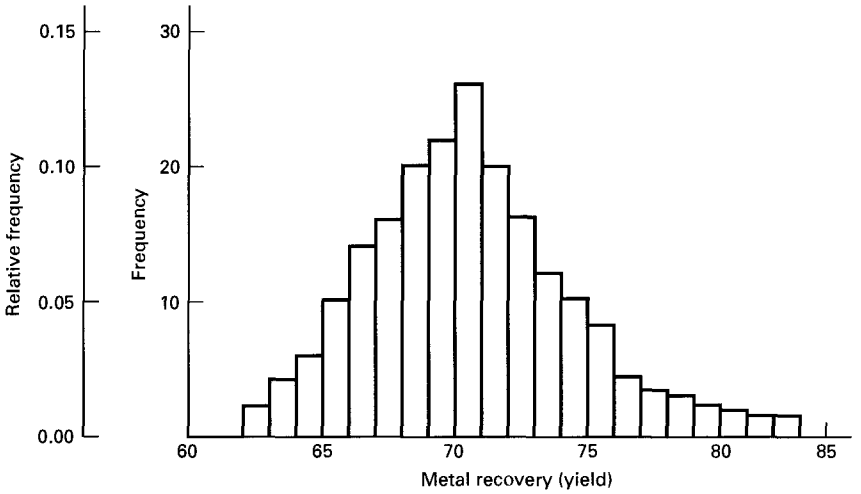


Figure 2-2 Histogram for 200 observations on metal recovery (yield) from a smelting process.

reveals that the two formulations probably differ in mean strength but that both formulations produce about the same variation in strength.

If the data are fairly numerous, the dots in a dot diagram become difficult to distinguish, and a histogram may be preferable. Figure 2-2 presents a histogram for 200 observations on the metal recovery, or yield, from a smelting process. The histogram shows the central tendency, spread, and general shape of the distribution of the data. Recall that a histogram is constructed by dividing the horizontal axis into intervals (usually of equal length) and drawing a rectangle over the jth interval with the area of the rectangle proportional to n_j, the number of observations that fall in that interval.

The **box plot** (or **box and whisker plot**) is a very useful way to display data. A box plot displays the minimum, the maximum, the lower and upper quartiles (the 25th percentile and the 75th percentile, respectively), and the median (the 50th percentile) on a rectangular box aligned either horizontally or vertically. The box extends from the lower quartile to the upper quartile, and a line is drawn through the box at the median. Lines (or whiskers) extend from the ends of the box to (typically) the minimum and maximum values. [There are several variations of box plots that have different rules for denoting the extreme sample points. See Montgomery and Runger (1999) for more details.]

Figure 2-3 (page 24) presents the box plots for the two samples of tension bond strength in the portland cement mortar experiment. This display clearly reveals the difference in mean strength between the two formulations. It also indicates that both formulations produce reasonably symmetric distributions of strength with similar variability or spread.

Dot diagrams, histograms, and box plots are useful for summarizing the information in a **sample** of data. To describe the observations that might occur in a sample more completely, we use the concept of the probability distribution.

Probability Distributions

The probability structure of a random variable, say y, is described by its **probability distribution**. If y is discrete, we often call the probability distribution of y, say $p(y)$, the

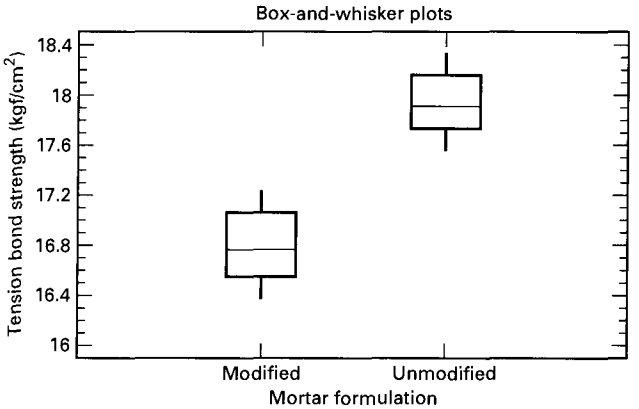
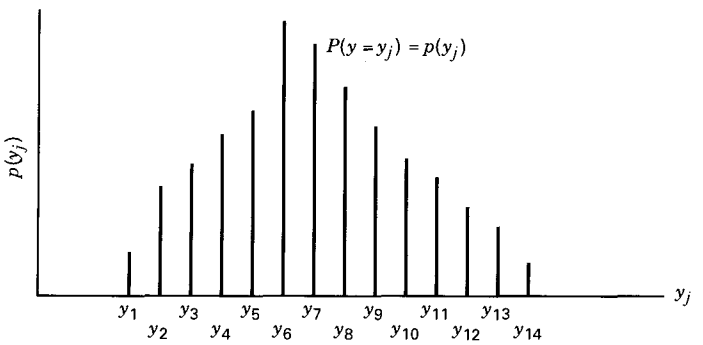


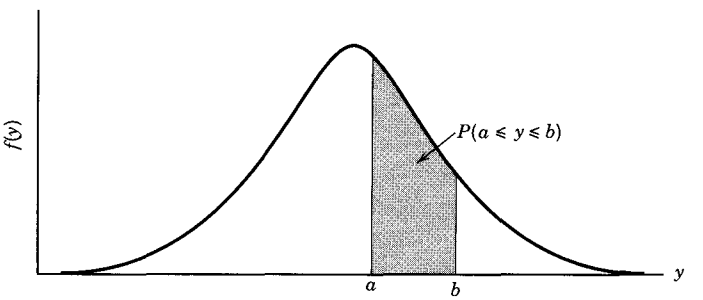
Figure 2-3 Box plots for the portland cement tension bond strength experiment.

probability function of y. If y is continuous, the probability distribution of y, say $f(y)$, is often called the probability density function for y.

Figure 2-4 illustrates hypothetical discrete and continuous probability distributions. Notice that in the discrete probability distribution, it is the height of the function $p(y_j)$ that represents probability, whereas in the continuous case, it is the area under the curve



(*a*) A discrete distribution



(*b*) A continuous distribution

Figure 2-4 Discrete and continuous probability distributions.

$f(y)$ associated with a given interval that represents probability. The properties of probability distributions may be summarized quantitatively as follows:

$$y \text{ discrete:} \quad 0 \leq p(y_j) \leq 1 \quad \text{all values of } y_j$$

$$P(y = y_j) = p(y_j) \quad \text{all values of } y_j$$

$$\sum_{\substack{\text{all values} \\ \text{of } y_j}} p(y_j) = 1$$

$$y \text{ continuous:} \quad 0 \leq f(y)$$

$$P(a \leq y \leq b) = \int_a^b f(y)\, dy$$

$$\int_{-\infty}^{\infty} f(y)\, dy = 1$$

Mean, Variance, and Expected Values

The **mean**, μ, of a probability distribution is a measure of its central tendency or location. Mathematically, we define the mean as

$$\mu = \begin{cases} \displaystyle\int_{-\infty}^{\infty} yf(y)\, dy & y \text{ continuous} \\ \displaystyle\sum_{\text{all } y} yp(y) & y \text{ discrete} \end{cases} \tag{2-1}$$

We may also express the mean in terms of the **expected value** or the long-run average value of the random variable y as

$$\mu = E(y) = \begin{cases} \displaystyle\int_{-\infty}^{\infty} yf(y)\, dy & y \text{ continuous} \\ \displaystyle\sum_{\text{all } y} yp(y) & y \text{ discrete} \end{cases} \tag{2-2}$$

where E denotes the **expected value operator**.

The variability or dispersion of a probability distribution can be measured by the **variance**, defined as

$$\sigma^2 = \begin{cases} \displaystyle\int_{-\infty}^{\infty} (y - \mu)^2 f(y)\, dy & y \text{ continuous} \\ \displaystyle\sum_{\text{all } y} (y - \mu)^2 p(y) & y \text{ discrete} \end{cases} \tag{2-3}$$

Note that the variance can be expressed entirely in terms of expectation because

$$\sigma^2 = E[(y - \mu)^2] \tag{2-4}$$

Finally, the variance is used so extensively that it is convenient to define a **variance operator** V such that

$$V(y) \equiv E[(y - \mu)^2] = \sigma^2 \tag{2-5}$$

The concepts of expected value and variance are used extensively throughout this book, and it may be helpful to review several elementary results concerning these operators. If y is a random variable with mean μ and variance σ^2 and c is a constant, then

1. $E(c) = c$
2. $E(y) = \mu$
3. $E(cy) = cE(y) = c\mu$
4. $V(c) = 0$
5. $V(y) = \sigma^2$
6. $V(cy) = c^2V(y) = c^2\sigma^2$

If there are two random variables, for example, y_1 with $E(y_1) = \mu_1$ and $V(y_1) = \sigma_1^2$ and y_2 with $E(y_2) = \mu_2$ and $V(y_2) = \sigma_2^2$, we have

7. $E(y_1 + y_2) = E(y_1) + E(y_2) = \mu_1 + \mu_2$

It is possible to show that

8. $V(y_1 + y_2) = V(y_1) + V(y_2) + 2\,\text{Cov}(y_1, y_2)$

where

$$\text{Cov}(y_1, y_2) = E[(y_1 - \mu_1)(y_2 - \mu_2)] \tag{2-6}$$

is the **covariance** of the random variables y_1 and y_2. The covariance is a measure of the linear association between y_1 and y_2. More specifically, we may show that if y_1 and y_2 are independent,[1] then $\text{Cov}(y_1, y_2) = 0$. We may also show that

9. $V(y_1 - y_2) = V(y_1) + V(y_2) - 2\,\text{Cov}(y_1, y_2)$

If y_1 and y_2 are **independent**, we have

10. $V(y_1 \pm y_2) = V(y_1) + V(y_2) = \sigma_1^2 + \sigma_2^2$

and

11. $E(y_1 \cdot y_2) = E(y_1) \cdot E(y_2) = \mu_1 \cdot \mu_2$

However, note that, in general,

12. $E\left(\dfrac{y_1}{y_2}\right) \neq \dfrac{E(y_1)}{E(y_2)}$

regardless of whether or not y_1 and y_2 are independent.

2-3 SAMPLING AND SAMPLING DISTRIBUTIONS

Random Samples, Sample Mean, and Sample Variance

The objective of statistical inference is to draw conclusions about a population using a sample from that population. Most of the methods that we will study assume that random

[1] Note that the converse of this is not necessarily so; that is, we may have $\text{Cov}(y_1, y_2) = 0$ and yet this does not imply independence. For an example, see Hines and Montgomery (1990, pp. 128–129).

samples are used. That is, if the population contains N elements and a sample of n of them is to be selected, and if each of the $N!/(N - n)!n!$ possible samples has an equal probability of being chosen, then the procedure employed is called **random sampling**. In practice, it is sometimes difficult to obtain random samples, and tables of random numbers, such as Table XI in the Appendix, may be helpful.

Statistical inference makes considerable use of quantities computed from the observations in the sample. We define a **statistic** as any function of the observations in a sample that does not contain unknown parameters. For example, suppose that $y_1, y_2, \ldots, y_n$ represents a sample. Then the **sample mean**

$$\bar{y} = \frac{\sum_{i=1}^{n} y_i}{n} \tag{2-7}$$

and the **sample variance**

$$S^2 = \frac{\sum_{i=1}^{n} (y_i - \bar{y})^2}{n - 1} \tag{2-8}$$

are both statistics. These quantities are measures of the central tendency and dispersion of the sample, respectively. Sometimes $S = \sqrt{S^2}$, called the **sample standard deviation**, is used as a measure of dispersion. Engineers often prefer to use the standard deviation to measure dispersion because its units are the same as those for the variable of interest y.

Properties of the Sample Mean and Variance

The sample mean $\bar{y}$ is a point estimator of the population mean μ, and the sample variance S^2 is a point estimator of the population variance σ^2. In general, an **estimator** of an unknown parameter is a statistic that corresponds to that parameter. Note that a point estimator is a random variable. A particular numerical value of an estimator, computed from sample data, is called an **estimate**. For example, suppose we wish to estimate the mean and variance of the breaking strength of a particular type of textile fiber. A random sample of $n = 25$ fiber specimens is tested and the breaking strength is recorded for each. The sample mean and variance are computed according to Equations 2-7 and 2-8, respectively, and are $\bar{y} = 18.6$ and $S^2 = 1.20$. Therefore, the estimate of μ is $\bar{y} = 18.6$ and the estimate of σ^2 is $S^2 = 1.20$.

There are several properties required of good point estimators. Two of the most important are the following:

1. The point estimator should be **unbiased**. That is, the long-run average or expected value of the point estimator should be the parameter that is being estimated. Although unbiasedness is desirable, this property alone does not always make an estimator a good one.
2. An unbiased estimator should have **minimum variance**. This property states that the minimum variance point estimator has a variance that is smaller than the variance of any other estimator of that parameter.

We may easily show that $\bar{y}$ and S^2 are unbiased estimators of μ and σ^2, respectively. First consider $\bar{y}$. Using the properties of expectation, we have

$$\begin{aligned} E(\bar{y}) &= E\left(\frac{\sum_{i=1}^{n} y_i}{n}\right) \\ &= \frac{1}{n} E\left(\sum_{i=1}^{n} y_i\right) \\ &= \frac{1}{n} \sum_{i=1}^{n} E(y_i) \\ &= \frac{1}{n} \sum_{i=1}^{n} \mu \\ &= \mu \end{aligned}$$

because the expected value of each observation y_i is μ. Thus, $\bar{y}$ is an unbiased estimator of μ.

Now consider the sample variance S^2. We have

$$\begin{aligned} E(S^2) &= E\left[\frac{\sum_{i=1}^{n} (y_i - \bar{y})^2}{n-1}\right] \\ &= \frac{1}{n-1} E\left[\sum_{i=1}^{n} (y_i - \bar{y})^2\right] \\ &= \frac{1}{n-1} E(SS) \end{aligned}$$

where $SS = \Sigma_{i=1}^{n}(y_i - \bar{y})^2$ is the **corrected sum of squares** of the observations y_i. Now

$$E(SS) = E\left[\sum_{i=1}^{n} (y_i - \bar{y})^2\right] \tag{2-9}$$

$$= E\left[\sum_{i=1}^{n} y_i^2 - n\bar{y}^2\right]$$

$$= \sum_{i=1}^{n} (\mu^2 + \sigma^2) - n(\mu^2 + \sigma^2/n)$$

$$= (n-1)\sigma^2 \tag{2-10}$$

Therefore,

$$\begin{aligned} E(S^2) &= \frac{1}{n-1} E(SS) \\ &= \sigma^2 \end{aligned}$$

and we see that S^2 is an unbiased estimator of σ^2.

Degrees of Freedom

The quantity $n - 1$ in Equation 2-10 is called the **number of degrees of freedom** of the sum of squares SS. This is a very general result; that is, if y is a random variable with variance σ^2 and $SS = \Sigma(y_i - \bar{y})^2$ has v degrees of freedom, then

$$E\left(\frac{SS}{v}\right) = \sigma^2 \tag{2-11}$$

The number of degrees of freedom of a sum of squares is equal to the number of independent elements in that sum of squares. For example, $SS = \Sigma_{i=1}^{n}(y_i - \bar{y})^2$ in Equation 2-9 consists of the sum of squares of the n elements $y_1 - \bar{y}, y_2 - \bar{y}, \ldots, y_n - \bar{y}$. These elements are not all independent because $\Sigma_{i=1}^{n}(y_i - \bar{y}) = 0$; in fact, only $n - 1$ of them are independent, implying that SS has $n - 1$ degrees of freedom.

The Normal and Other Sampling Distributions

Often we are able to determine the probability distribution of a particular statistic if we know the probability distribution of the population from which the sample was drawn. The probability distribution of a statistic is called a **sampling distribution**. We will now briefly discuss several useful sampling distributions.

One of the most important sampling distributions is the **normal distribution**. If y is a normal random variable, the probability distribution of y is

$$f(y) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(1/2)[(y-\mu)/\sigma]^2} \qquad -\infty < y < \infty \tag{2-12}$$

where $-\infty < \mu < \infty$ is the mean of the distribution and $\sigma^2 > 0$ is the variance. The normal distribution is shown in Figure 2-5.

Because sample runs that differ as a result of experimental error often are well described by the normal distribution, the normal plays a central role in the analysis of data from designed experiments. Many important sampling distributions may also be defined in terms of normal random variables. We often use the notation $y \sim N(\mu, \sigma^2)$ to denote that y is distributed normally with mean μ and variance σ^2.

An important special case of the normal distribution is the **standard normal distribution**; that is, $\mu = 0$ and $\sigma^2 = 1$. We see that if $y \sim N(\mu, \sigma^2)$, the random variable

$$z = \frac{y - \mu}{\sigma} \tag{2-13}$$

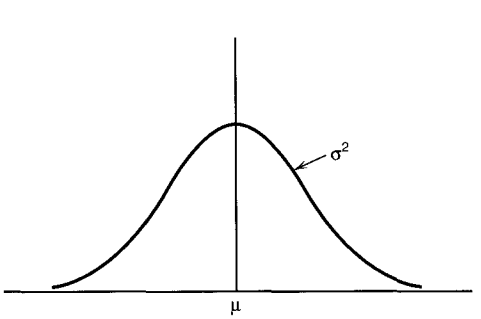


Figure 2-5 The normal distribution.

follows the standard normal distribution, denoted $z \sim N(0, 1)$. The operation demonstrated in Equation 2-13 is often called **standardizing** the normal random variable y. The cumulative standard normal distribution is given in Table I of the Appendix.

Many statistical techniques assume that the random variable is normally distributed. The central limit theorem is often a justification of approximate normality.

THEOREM 2-1

The Central Limit Theorem

If $y_1, y_2, \ldots, y_n$ is a sequence of n independent and identically distributed random variables with $E(y_i) = \mu$ and $V(y_i) = \sigma^2$ (both finite) and $x = y_1 + y_2 + \cdots + y_n$, then

$$z_n = \frac{x - n\mu}{\sqrt{n\sigma^2}}$$

has an approximate $N(0, 1)$ distribution in the sense that, if $F_n(z)$ is the distribution function of z_n and $\Phi(z)$ is the distribution function of the $N(0, 1)$ random variable, then $\lim_{n\to\infty}[F_n(z)/\Phi(z)] = 1$.

This result states essentially that the sum of n independent and identically distributed random variables is approximately normally distributed. In many cases this approximation is good for very small n, say $n < 10$, whereas in other cases large n is required, say $n > 100$. Frequently, we think of the error in an experiment as arising in an additive manner from several independent sources; consequently, the normal distribution becomes a plausible model for the combined experimental error.

An important sampling distribution that can be defined in terms of normal random variables is the **chi-square** or χ^2 **distribution**. If $z_1, z_2, \ldots, z_k$ are normally and independently distributed random variables with mean 0 and variance 1, abbreviated NID(0, 1), then the random variable

$$x = z_1^2 + z_2^2 + \cdots + z_k^2$$

follows the chi-square distribution with k degrees of freedom. The density function of chi-square is

$$f(x) = \frac{1}{2^{k/2}\Gamma\left(\frac{k}{2}\right)} x^{(k/2)-1}e^{-x/2} \qquad x > 0 \tag{2-14}$$

Several chi-square distributions are shown in Figure 2-6. The distribution is asymmetric, or **skewed**, with mean and variance

$$\mu = k$$
$$\sigma^2 = 2k$$

respectively. Percentage points of the chi-square distribution are given in Table III of the Appendix.

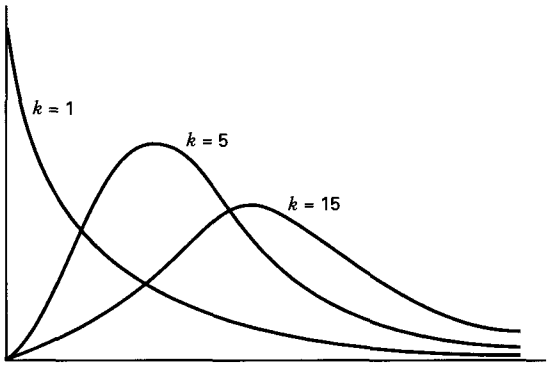


Figure 2-6 Several chi-square distributions.

As an example of a random variable that follows the chi-square distribution, suppose that $y_1, y_2, \ldots, y_n$ is a random sample from an $N(\mu, \sigma^2)$ distribution. Then

$$\frac{SS}{\sigma^2} = \frac{\sum_{i=1}^{n} (y_i - \bar{y})^2}{\sigma^2} \sim \chi^2_{n-1} \tag{2-15}$$

That is, SS/σ^2 is distributed as chi-square with $n - 1$ degrees of freedom.

Many of the techniques used in this book involve the computation and manipulation of sums of squares. The result given in Equation 2-15 is extremely important and occurs repeatedly; a sum of squares in normal random variables when divided by σ^2 follows the chi-square distribution.

Examining Equation 2-8, we see that the sample variance can be written as

$$S^2 = \frac{SS}{n - 1} \tag{2-16}$$

If the observations in the sample are NID(μ, σ^2), then the distribution of S^2 is $[\sigma^2/(n - 1)]\chi^2_{n-1}$. Thus, the sampling distribution of the sample variance is a constant times the chi-square distribution if the population is normally distributed.

If z and χ^2_k are independent standard normal and chi-square random variables, respectively, the random variable

$$t_k = \frac{z}{\sqrt{\chi^2_k/k}} \tag{2-17}$$

follows the ***t* distribution with *k* degrees of freedom**, denoted t_k. The density function of t is

$$f(t) = \frac{\Gamma[(k + 1)/2]}{\sqrt{k\pi}\Gamma(k/2)} \frac{1}{[(t^2/k) + 1]^{(k+1)/2}} \qquad -\infty < t < \infty \tag{2-18}$$

and the mean and variance of t are $\mu = 0$ and $\sigma^2 = k/(k - 2)$ for $k > 2$, respectively. Several t distributions are shown in Figure 2-7 on page 32. Note that if $k = \infty$, the t distribution becomes the standard normal distribution. The percentage points of the t

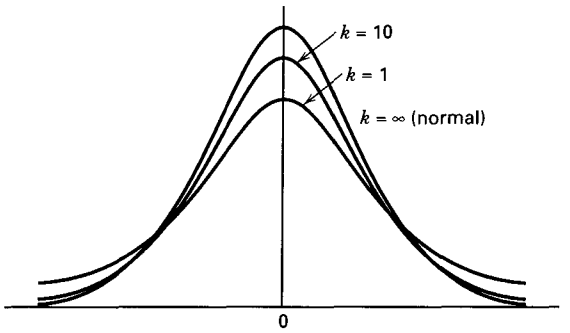


Figure 2-7 Several t distributions.

distribution are given in Table II of the Appendix. If $y_1, y_2, \ldots, y_n$ is a random sample from the $N(\mu, \sigma^2)$ distribution, then the quantity

$$t = \frac{\bar{y} - \mu}{S/\sqrt{n}} \tag{2-19}$$

is distributed as t with $n - 1$ degrees of freedom.

The final sampling distribution that we will consider is the ***F* distribution**. If χ_u^2 and χ_v^2 are two independent chi-square random variables with u and v degrees of freedom, respectively, then the ratio

$$F_{u,v} = \frac{\chi_u^2/u}{\chi_v^2/v} \tag{2-20}$$

follows the F distribution with u *numerator* degrees of freedom and v *denominator* degrees of freedom. If x is an F random variable with u numerator and v denominator degrees of freedom, then the probability distribution of x is

$$h(x) = \frac{\Gamma\left(\frac{u+v}{2}\right)\left(\frac{u}{v}\right)^{u/2} x^{(u/2)-1}}{\Gamma\left(\frac{u}{2}\right)\Gamma\left(\frac{v}{2}\right)\left[\left(\frac{u}{v}\right)x + 1\right]^{(u+v)/2}} \qquad 0 < x < \infty \tag{2-21}$$

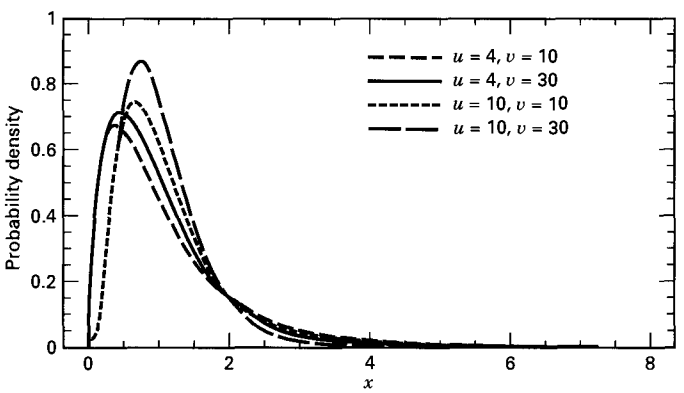


Figure 2-8 Several F distributions.

Several F distributions are shown in Figure 2-8 on the preceding page. This distribution is very important in the statistical analysis of designed experiments. Percentage points of the F distribution are given in Table IV of the Appendix.

As an example of a statistic that is distributed as F, suppose we have two independent normal populations with common variance σ^2. If $y_{11}, y_{12}, \ldots, y_{1n_1}$, is a random sample of n_1 observations from the first population, and if $y_{21}, y_{22}, \ldots, y_{2n_2}$ is a random sample of n_2 observations from the second, then

$$\frac{S_1^2}{S_2^2} \sim F_{n_1-1,n_2-1} \tag{2-22}$$

where S_1^2 and S_2^2 are the two sample variances. This result follows directly from Equations 2-15 and 2-20.

2-4 INFERENCES ABOUT THE DIFFERENCES IN MEANS, RANDOMIZED DESIGNS

We are now ready to return to the portland cement mortar problem posed in Section 2-1. Recall that two different formulations of mortar were being investigated to determine if they differ in tension bond strength. In this section we discuss how the data from this simple comparative experiment can be analyzed using **hypothesis testing** and **confidence interval** procedures for comparing two treatment means.

Throughout this section we assume that a **completely randomized experimental design** is used. In such a design, the data are viewed as if they were a random sample from a normal distribution.

2-4.1 Hypothesis Testing

We now reconsider the portland cement experiment introduced in Section 2-1. Recall that we are interested in comparing the strength of two different formulations: an unmodified mortar and a modified mortar. In general, we can think of these two formulations as two **levels of the factor** "formulations." Let $y_{11}, y_{12}, \ldots, y_{1n_1}$ represent the n_1 observations from the first factor level and $y_{21}, y_{22}, \ldots, y_{2n_2}$ represent the n_2 observations from the second factor level. We assume that the samples are drawn at random from two independent normal populations. Figure 2-9 illustrates the situation.

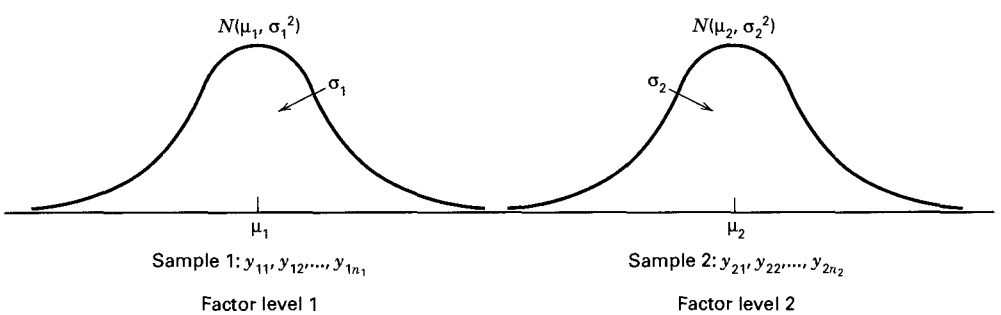


Figure 2-9 The sampling situation for the two-sample t-test.

A Model for the Data

We often describe the results of an experiment with a **model**. A simple statistical model that describes the data from an experiment such as we have just described is

$$y_{ij} = \mu_i + \varepsilon_{ij} \begin{cases} i = 1,2 \\ j = 1, 2, \ldots, n_i \end{cases} \tag{2-23}$$

where y_{ij} is the jth observation from factor level i, μ_i is the mean of the response at the ith factor level, and ε_{ij} is a normal random variable associated with the ijth observation. We assume that ε_{ij} are NID(0, σ_i^2), $i = 1, 2$. It is customary to refer to ε_{ij} as the **random error** component of the model. Because the means μ_1 and μ_2 are constants, we see directly from the model that y_{ij} are NID(μ_i, σ_i^2), $i = 1, 2$, just as we previously assumed. For more information about models for the data, refer to the supplemental text material.

Statistical Hypotheses

A **statistical hypothesis** is a statement either about the parameters of a probability distribution or the parameters of a model. The hypothesis reflects some **conjecture** about the problem situation. For example, in the portland cement experiment, we may think that the mean tension bond strengths of the two mortar formulations are equal. This may be stated formally as

$$H_0: \mu_1 = \mu_2$$
$$H_1: \mu_1 \neq \mu_2$$

where μ_1 is the mean tension bond strength of the modified mortar and μ_2 is the mean tension bond strength of the unmodified mortar. The statement $H_0: \mu_1 = \mu_2$ is called the **null hypothesis** and $H_1: \mu_1 \neq \mu_2$ is called the **alternative hypothesis**. The alternative hypothesis specified here is called a **two-sided alternative hypothesis** because it would be true if $\mu_1 < \mu_2$ or if $\mu_1 > \mu_2$.

To test a hypothesis we devise a procedure for taking a random sample, computing an appropriate **test statistic**, and then rejecting or failing to reject the null hypothesis H_0. Part of this procedure is specifying the set of values for the test statistic that leads to rejection of H_0. This set of values is called the **critical region** or **rejection region** for the test.

Two kinds of errors may be committed when testing hypotheses. If the null hypothesis is rejected when it is true, a type I error has occurred. If the null hypothesis is *not* rejected when it is false, a type II error has been made. The probabilities of these two errors are given special symbols:

$$\alpha = P(\text{type I error}) = P(\text{reject } H_0 | H_0 \text{ is true})$$
$$\beta = P(\text{type II error}) = P(\text{fail to reject } H_0 | H_0 \text{ is false})$$

Sometimes it is more convenient to work with the **power** of the test, where

$$\text{Power} = 1 - \beta = P(\text{reject } H_0 | H_0 \text{ is false})$$

The general procedure in hypothesis testing is to specify a value of the probability of type I error α, often called the **significance level** of the test, and then design the test procedure so that the probability of type II error β has a suitably small value.

The Two-Sample *t*-Test

Suppose that we could assume that the variances of tension bond strengths were identical for both mortar formulations. Then the appropriate test statistic to use for comparing two treatment means in the completely randomized design is

$$t_0 = \frac{\bar{y}_1 - \bar{y}_2}{S_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \tag{2-24}$$

where $\bar{y}_1$ and $\bar{y}_2$ are the sample means, n_1 and n_2 are the sample sizes, S_p^2 is an estimate of the common variance $\sigma_1^2 = \sigma_2^2 = \sigma^2$ computed from

$$S_p^2 = \frac{(n_1 - 1)S_1^2 + (n_2 - 1)S_2^2}{n_1 + n_2 - 2} \tag{2-25}$$

and S_1^2 and S_2^2 are the two individual sample variances. To determine whether to reject $H_0: \mu_1 = \mu_2$, we would compare t_0 to the t distribution with $n_1 + n_2 - 2$ degrees of freedom. If $|t_0| > t_{\alpha/2,n_1+n_2-2}$, where $t_{\alpha/2,n_1+n_2-2}$ is the upper $\alpha/2$ percentage point of the t distribution with $n_1 + n_2 - 2$ degrees of freedom, we would *reject* H_0 and conclude that the mean strengths of the two formulations of portland cement mortar differ. This test procedure is usually called the **two-sample *t*-test**.

This procedure may be justified as follows. If we are sampling from independent normal distributions, then the distribution of $\bar{y}_1 - \bar{y}_2$ is $N[\mu_1 - \mu_2, \sigma^2(1/n_1 + 1/n_2)]$. Thus, if σ^2 were known, and if $H_0: \mu_1 = \mu_2$ were true, the distribution of

$$Z_0 = \frac{\bar{y}_1 - \bar{y}_2}{\sigma\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \tag{2-26}$$

would be $N(0, 1)$. However, in replacing σ in Equation 2-26 by S_p, the distribution of Z_0 changes from standard normal to t with $n_1 + n_2 - 2$ degrees of freedom. Now if H_0 is true, t_0 in Equation 2-24 is distributed as $t_{n_1+n_2-2}$ and, consequently, we would expect $100(1 - \alpha)$ percent of the values of t_0 to fall between $-t_{\alpha/2,n_1+n_2-2}$ and $t_{\alpha/2,n_1+n_2-2}$. A sample producing a value of t_0 outside these limits would be unusual if the null hypothesis were true and is evidence that H_0 should be rejected. Thus the t distribution with $n_1 + n_2 - 2$ degrees of freedom is the appropriate **reference distribution** for the test statistic t_0. That is, it describes the behavior of t_0 when the null hypothesis is true. Note that α is the probability of type I error for the test.

In some problems, one may wish to reject H_0 only if one mean is larger than the other. Thus, one would specify a **one-sided alternative hypothesis** $H_1: \mu_1 > \mu_2$ and would reject H_0 only if $t_0 > t_{\alpha,n_1+n_2-2}$. If one wants to reject H_0 only if μ_1 is less than μ_2, then the alternative hypothesis is $H_1: \mu_1 < \mu_2$, and one would reject H_0 if $t_0 < -t_{\alpha,n_1+n_2-2}$.

To illustrate the procedure, consider the portland cement data in Table 2-1. For these data, we find that

Modified Mortar	Unmodified Mortar
$\bar{y}_1 = 16.76$ kgf/cm^2	$\bar{y}_2 = 17.92$ kgf/cm^2
$S_1^2 = 0.100$	$S_2^2 = 0.061$
$S_1 = 0.316$	$S_2 = 0.247$
$n_1 = 10$	$n_2 = 10$

Because the sample standard deviations are reasonably similar, it is not unreasonable to conclude that the population standard deviations (or variances) are equal. Therefore, we can use Equation 2-24 to test the hypotheses

$$H_0: \mu_1 = \mu_2$$
$$H_1: \mu_1 \neq \mu_2$$

Furthermore, $n_1 + n_2 - 2 = 10 + 10 - 2 = 18$, and if we choose $\alpha = 0.05$, then we would reject $H_0: \mu_1 = \mu_2$ if the numerical value of the test statistic $t_0 > t_{0.025,18} = 2.101$, or if $t_0 < -t_{0.025,18} = -2.101$. These boundaries of the critical region are shown on the reference distribution (t with 18 degrees of freedom) in Figure 2-10.

Using Equation 2-25 we find that

$$\begin{aligned} S_p^2 &= \frac{(n_1 - 1)S_1^2 + (n_2 - 1)S_2^2}{n_1 + n_2 - 2} \\ &= \frac{9(0.100) + 9(0.061)}{10 + 10 - 2} \\ &= 0.081 \\ S_p &= 0.284 \end{aligned}$$

and the test statistic is

$$\begin{aligned} t_0 &= \frac{\bar{y}_1 - \bar{y}_2}{S_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \\ &= \frac{16.76 - 17.92}{0.284\sqrt{\frac{1}{10} + \frac{1}{10}}} \\ &= -9.13 \end{aligned}$$

Because $t_0 = -9.13 < -t_{0.025,18} = -2.101$, we would reject H_0 and conclude that the mean tension bond strengths of the two formulations of portland cement mortar are different.

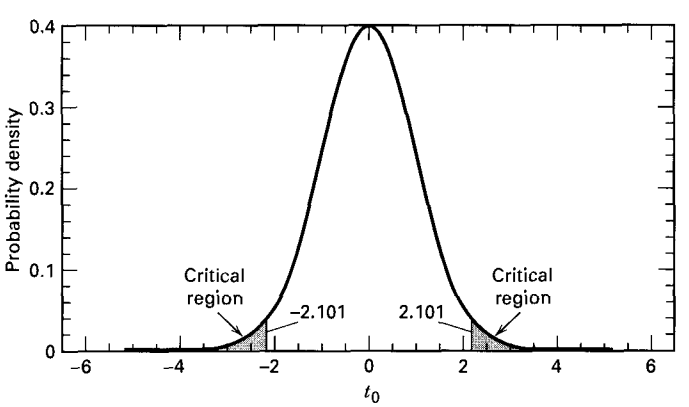


Figure 2-10 The t distribution with 18 degrees of freedom with the critical region $\pm t_{0.025,18} = \pm 2.101$.

The Use of *P*-Values in Hypothesis Testing

One way to report the results of a hypothesis test is to state that the null hypothesis was or was not rejected at a specified α-value or **level of significance**. For example, in the portland cement mortar formulation above, we can say that $H_0: \mu_1 = \mu_2$ was rejected at the 0.05 level of significance. This statement of conclusions is often inadequate because it gives the decision maker no idea about whether the computed value of the test statistic was just barely in the rejection region or whether it was very far into this region. Furthermore, stating the results this way imposes the predefined level of significance on other users of the information. This approach may be unsatisfactory because some decision makers might be uncomfortable with the risks implied by $\alpha = 0.05$.

To avoid these difficulties, the ***P*-value approach** has been adopted widely in practice. The *P*-value is the probability that the test statistic will take on a value that is at least as extreme as the observed value of the statistic when the null hypothesis H_0 is true. Thus, a *P*-value conveys much information about the weight of evidence against H_0, and so a decision maker can draw a conclusion at *any* specified level of significance. More formally, we define the ***P*-value** as the smallest level of significance that would lead to rejection of the null hypothesis H_0.

It is customary to call the test statistic (and the data) significant when the null hypothesis H_0 is rejected; therefore, we may think of the *P*-value as the smallest level α at which the data are significant. Once the *P*-value is known, the decision maker can determine how significant the data are without the data analyst formally imposing a preselected level of significance.

It is not always easy to compute the exact *P*-value for a test. However, most modern computer programs for statistical analysis report *P*-values, and they can be obtained on some handheld calculators. We will show how to approximate the *P*-value for the portland cement mortar experiment. From Appendix Table II, for a t distribution with 18 degrees of freedom, the smallest tail area probability is 0.0005, for which $t_{0.0005,18} = 3.922$. Now $|t_0| = 9.13 > 3.922$, so because the alternative hypothesis is two-sided, we know that the *P*-value must be less than $2(0.0005) = 0.001$. Some handheld calculators have the capability to calculate *P*-values. One such calculator is the HP-48. From this calculator, we obtain the *P*-value for the value $t_0 = -9.13$ in the portland cement mortar formulation experiment as $P = 3.68 \times 10^{-8}$. Thus the null hypothesis $H_0: \mu_1 = \mu_2$ would be rejected at any level of significance $\alpha \geq 3.68 \times 10^{-8}$.

Computer Solution

There are many statistical software packages that have capability for statistical hypothesis testing. The output from the Minitab two-sample t-test procedure applied to the portland cement mortar formulation experiment is shown in Table 2-2 on the next page. Notice that the output includes some summary statistics about the two samples (the abbreviation "SE mean" refers to the standard error of the mean, $s/\sqrt{n}$) as well as some information about confidence intervals on the difference in the two means (which we will discuss in Sections 2-4.3 and 2-6). The program also tests the hypothesis of interest, allowing the analyst to specify the nature of the alternative hypothesis ("not =" implies $H_1: \mu_1 \neq \mu_2$) and the choice of α (here $\alpha = 0.05$).

The output includes the computed value of t_0, the *P*-value (called the significance level), and the decision that should be made given the specified value of α. Notice that the computed value of the t statistic differs slightly from our manually calculated value and that the *P*-value is reported to be $P = 0.0000$. Many software packages will not

Table 2-2 Minitab Two-Sample *t*-Test for the Portland Cement Mortar Experiment

Two Sample *t*-Test and Confidence Interval

```
Two sample T for Modified vs Unmod

              N       Mean      StDev     SE Mean
Modified     10     16.774      0.309        0.098
Unmod        10     17.922      0.248        0.078

95% CI for mu Modified - mu Unmod: ( -1.411,  -0.885)
t-Test mu Modified = mu Unmod (vs not =): T = -9.16
P = 0.0000 DF = 18
Both use Pooled StDev = 0.280
```

report an actual *P*-value less than 0.0001 and instead return a "default" value. That is the case here.

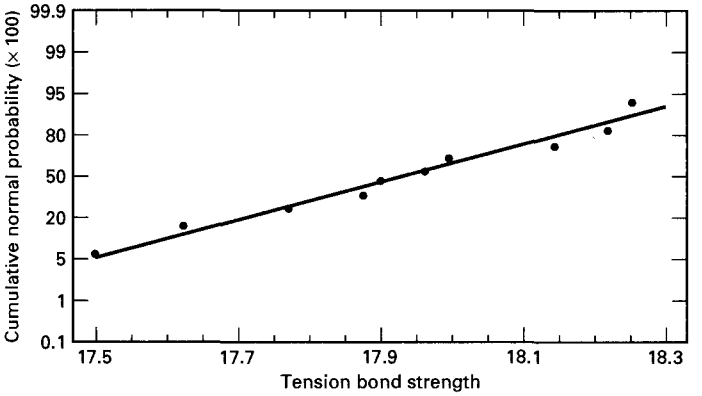
Checking Assumptions in the *t*-Test

In using the *t*-test procedure we make the assumptions that both samples are drawn from independent populations that can be described by a normal distribution, that the standard deviation or variances of both populations are equal, and that the observations are independent random variables. The assumption of independence is critical, and if the run order is randomized (and, if appropriate, other experimental units and materials are selected at random), this assumption will usually be satisfied. The equal-variance and normality assumptions are easy to check using a **normal probability plot**.

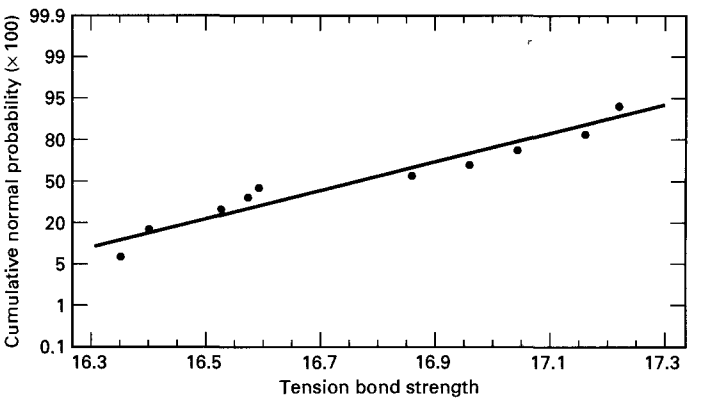
Generally, probability plotting is a graphical technique for determining whether sample data conform to a hypothesized distribution based on a subjective visual examination of the data. The general procedure is very simple and can be performed quickly with most statistics software packages. The supplemental text material discusses manual construction of normal probability plots.

To construct a probability plot, the observations in the sample are first ranked from smallest to largest. That is, the sample $y_1, y_2, \ldots, y_n$ is arranged as $y_{(1)}, y_{(2)}, \ldots, y_{(n)}$ where $y_{(1)}$ is the smallest observation, $y_{(2)}$ is the second smallest observation, and so forth, with $y_{(n)}$ the largest. The ordered observations $y_{(j)}$ are then plotted against their observed cumulative frequency $(j - 0.5)/n$. The cumulative frequency scale has been arranged so that if the hypothesized distribution adequately describes the data, the plotted points will fall approximately along a straight line; if the plotted points deviate significantly from a straight line, the hypothesized model is not appropriate. Usually, the determination of whether or not the data plot as a straight line is subjective.

To illustrate the procedure, suppose that we wish to check the assumption that tension bond strength in the portland cement mortar formulation experiment is normally distributed. We initially consider only the observations from the unmodified mortar formulation. A computer-generated normal probability plot is shown in Figure 2-11*a*. Most normal probability plots present $100(j - 0.5)/n$ on the left vertical scale (and occasionally $100[1 - (j - 0.5)/n]$ is plotted on the right vertical scale), with the variable value plotted on the horizontal scale. Some computer-generated normal probability plots convert the cumulative frequency to a standard normal z score. A straight line, chosen subjectively, has been drawn through the plotted points. In drawing the straight line, you should be



(*a*) Unmodified mortar



(*b*) Modified mortar

Figure 2-11 Normal probability plots of tension bond strength in the portland cement experiment.

influenced more by the points near the middle of the plot than by the extreme points. A good rule of thumb is to draw the line approximately between the 25th and 75th percentile points. This is how the line in Figure 2-11*a* was determined. In assessing the "closeness" of the points to the straight line, imagine a fat pencil lying along the line. If all the points are covered by this imaginary pencil, a normal distribution adequately describes the data. Because the points in Figure 2-11*a* would pass the fat pencil test, we conclude that the normal distribution is an appropriate model for tension bond strength for the unmodified mortar. Figure 2-11*b* presents the normal probability plot for the 10 observations on tension bond strength for the modified mortar. Once again, we would conclude that the assumption of a normal distribution is reasonable.

We can obtain an estimate of the mean and standard deviation directly from the normal probability plot. The mean is estimated as the 50th percentile on the probability plot, and the standard deviation is estimated as the difference between the 84th and 50th percentiles. This means that we can verify the assumption of equal population variances in the portland cement experiment by simply comparing the slopes of the two straight lines in Figure 2-11*a* and 2-11*b*. Both lines have very similar slopes, and so the as-

sumption of equal variances is a reasonable one. If this assumption is violated, you should use the version of the t-test described in Section 2-4.4. The supplemental text material has more information about checking assumptions on the t-test.

When assumptions are badly violated, the performance of the t-test will be affected. Generally, small to moderate violations of assumptions are not a major concern, but *any* failure of the independence assumption and strong indications of nonnormality should not be ignored. Both the significance level of the test and the ability to detect differences between the means will be adversely affected by departures from assumptions. **Transformations** are one approach to dealing with this problem. We will discuss this in more detail in Chapter 3. Nonparametric hypothesis testing procedures can also be used if the observations come from nonnormal populations. Refer to Montgomery and Runger (1999) for more details.

An Alternate Justification to the t-Test

The two-sample t-test we have just presented depends in theory on the underlying assumption that the two populations from which the samples were randomly selected are normal. Although the normality assumption is required to develop the test procedure formally, as we discussed above, moderate departures from normality will not seriously affect the results. It can be argued [e.g., see Box, Hunter, and Hunter (1978)] that the use of a randomized design enables one to test hypotheses without *any* assumptions regarding the form of the distribution. Briefly, the reasoning is as follows. If the treatments have no effect, all $[20!/(10!10!)] = 184{,}756$ possible ways that the 20 observations could occur are equally likely. Corresponding to each of these 184,756 possible arrangements is a value of t_0. If the value of t_0 actually obtained from the data is unusually large or unusually small with reference to the set of 184,756 possible values, it is an indication that $\mu_1 \neq \mu_2$.

This type of procedure is called a **randomization test**. It can be shown that the t-test is a good approximation of the randomization test. Thus, we will use t-tests (and other procedures that can be regarded as approximations of randomization tests) without extensive concern about the assumption of normality. This is one reason a simple procedure such as normal probability plotting is adequate to check the assumption of normality.

2-4.2 Choice of Sample Size

Selection of an appropriate sample size is one of the most important aspects of any experimental design problem. The choice of sample size and the probability of type II error β are closely connected. Suppose that we are testing the hypotheses

$$H_0: \mu_1 = \mu_2$$
$$H_1: \mu_1 \neq \mu_2$$

and that the means are *not* equal so that $\delta = \mu_1 - \mu_2$. Because $H_0: \mu_1 = \mu_2$ is not true, we are concerned about wrongly failing to reject H_0. The probability of type II error depends on the true difference in means δ. A graph of β versus δ for a particular sample size is called the **operating characteristic curve**, or **O.C. curve** for the test. The β error is also a function of sample size. Generally, for a given value of δ, the β error decreases as the sample size increases. That is, a specified difference in means is easier to detect for larger sample sizes than for smaller ones.

A set of operating characteristic curves for the hypotheses

$$H_0: \mu_1 = \mu_2$$
$$H_1: \mu_1 \neq \mu_2$$

for the case where the two population variances σ_1^2 and σ_2^2 are unknown but equal ($\sigma_1^2 = \sigma_2^2 = \sigma^2$) and for a level of significance of $\alpha = 0.05$ is shown in Figure 2-12. The curves also assume that the sample sizes from the two populations are equal; that is, $n_1 = n_2 = n$. The parameter on the horizontal axis in Figure 2-12 is

$$d = \frac{|\mu_1 - \mu_2|}{2\sigma} = \frac{|\delta|}{2\sigma}$$

Dividing $|\delta|$ by 2σ allows the experimenter to use the same set of curves, regardless of the value of the variance (the difference in means is expressed in standard deviation units). Furthermore, the sample size used to construct the curves is actually $n^* = 2n - 1$.

From examining these curves, we note the following:

1. The greater the difference in means, $\mu_1 - \mu_2$, the smaller the probability of type II error for a given sample size and α. That is, for a specified sample size and α, the test will detect large differences more easily than small ones.
2. As the sample size gets larger, the probability of type II error gets smaller for a given difference in means and α. That is, to detect a specified difference δ, we may make the test more powerful by increasing the sample size.

Operating characteristic curves are often helpful in selecting a sample size to use in an experiment. For example, consider the portland cement mortar problem discussed previously. Suppose that if the two formulations differ in mean strength by as much as 0.5 kgf/cm^2 we would like to detect it with a high probability. Thus, because $\mu_1 - \mu_2 =$

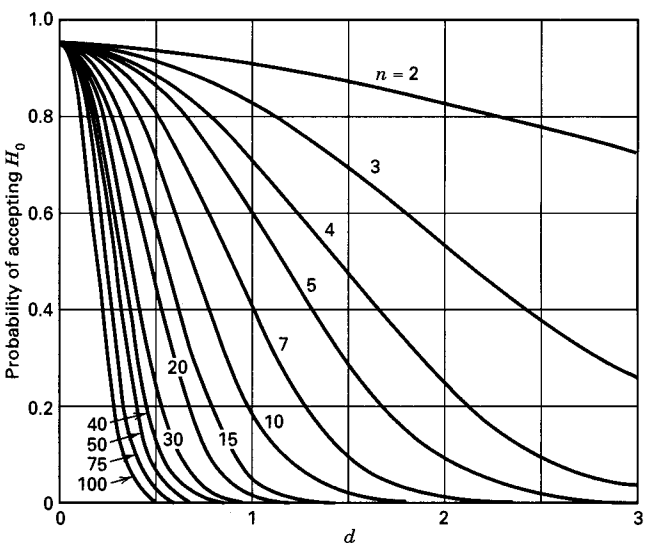


Figure 2-12 Operating characteristic curves for the two-sided t-test with $\alpha = 0.05$. (Reproduced with permission from "Operating Characteristics for the Common Statistical Tests of Significance," C. L. Ferris, F. E. Grubbs, and C. L. Weaver, *Annals of Mathematical Statistics*, June 1946.)

0.5 kgf/cm^2 is the "critical" difference in means we wish to detect, we find that d, the parameter on the horizontal axis of the operating characteristic curve in Figure 2-12, is

$$d = \frac{|\mu_1 - \mu_2|}{2\sigma} = \frac{0.5}{2\sigma} = \frac{0.25}{\sigma}$$

Unfortunately, d involves the unknown parameter σ. However, suppose that we think on the basis of prior experience that it is very unlikely that the standard deviation of any observation on strength would exceed 0.25 kgf/cm^2. Then using $\sigma = 0.25$ in the above expression for d yields $d = 1$. If we wish to reject the null hypothesis 95 percent of the time when $\mu_1 - \mu_2 = 0.5$, then $\beta = 0.05$, and Figure 2-12 with $\beta = 0.05$ and $d = 1$ yields $n^* = 16$, approximately. Therefore, because $n^* = 2n - 1$, the required sample size is

$$n = \frac{n^* + 1}{2} = \frac{16 + 1}{2} = 8.5 \simeq 9$$

and we would use sample sizes of $n_1 = n_2 = n = 9$.

In our example, the experimenter actually used a sample size of 10. Perhaps the experimenter elected to increase the sample size slightly to guard against the possibility that the prior estimate of the common standard deviation σ was too conservative and was likely to be somewhat larger than 0.25.

Operating characteristic curves often play an important role in the choice of sample size in experimental design problems. Their use in this respect is discussed in subsequent chapters. For a discussion of the uses of operating characteristic curves for other simple comparative experiments similar to the two-sample t-test see Montgomery and Runger (1999).

2-4.3 Confidence Intervals

Although hypothesis testing is a useful procedure, it sometimes does not tell the entire story. It is often preferable to provide an interval within which the value of the parameter or parameters in question would be expected to lie. These interval statements are called **confidence intervals**. In many engineering and industrial experiments, the experimenter already knows that the means μ_1 and μ_2 differ; consequently, hypothesis testing on $\mu_1 = \mu_2$ is of little interest. The experimenter would usually be more interested in a confidence interval on the difference in means $\mu_1 - \mu_2$.

To define a confidence interval, suppose that θ is an unknown parameter. To obtain an interval estimate of θ, we need to find two statistics L and U such that the probability statement

$$P(L \leq \theta \leq U) = 1 - \alpha \tag{2-27}$$

is true. The interval

$$L \leq \theta \leq U \tag{2-28}$$

is called a **100(1 − α) percent confidence interval** for the parameter θ. The interpretation of this interval is that if, in repeated random samplings, a large number of such intervals are constructed, 100(1 − α) percent of them will contain the true value of θ. The statistics L and U are called the **lower** and **upper confidence limits**, respectively,

and $1 - \alpha$ is called the **confidence coefficient**. If $\alpha = 0.05$, Equation 2-28 is called a 95 percent confidence interval for θ. Note that confidence intervals have a frequency interpretation; that is, we do not know if the statement is true for this specific sample, but we do know that the *method* used to produce the confidence interval yields correct statements $100(1 - \alpha)$ percent of the time.

Suppose that we wish to find a $100(1 - \alpha)$ percent confidence interval on the true difference in means $\mu_1 - \mu_2$ for the portland cement problem. The interval can be derived in the following way. The statistic

$$\frac{\bar{y}_1 - \bar{y}_2 - (\mu_1 - \mu_2)}{S_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}}$$

is distributed as $t_{n_1+n_2-2}$. Thus,

$$P\left(-t_{\alpha/2,n_1+n_2-2} \leq \frac{\bar{y}_1 - \bar{y}_2 - (\mu_1 - \mu_2)}{S_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \leq t_{\alpha/2,n_1+n_2-2}\right) = 1 - \alpha$$

or

$$P\left(\bar{y}_1 - \bar{y}_2 - t_{\alpha/2,n_1+n_2-2}S_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}} \leq \mu_1 - \mu_2 \leq \bar{y}_1 - \bar{y}_2 + t_{\alpha/2,n_1+n_2-2}S_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}\right) = 1 - \alpha \quad (2\text{-}29)$$

Comparing Equations 2-29 and 2-27, we see that

$$\bar{y}_1 - \bar{y}_2 - t_{\alpha/2,n_1+n_2-2}S_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}} \leq \mu_1 - \mu_2 \leq \bar{y}_1 - \bar{y}_2 + t_{\alpha/2,n_1+n_2-2}S_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}} \quad (2\text{-}30)$$

is a $100(1 - \alpha)$ percent confidence interval for $\mu_1 - \mu_2$.

The actual 95 percent confidence interval estimate for the difference in mean tension bond strength for the formulations of portland cement mortar is found by substituting in Equation 2-30 as follows:

$$16.76 - 17.92 - (2.101)0.284\sqrt{\tfrac{1}{10} + \tfrac{1}{10}} \leq \mu_1 - \mu_2 \leq 16.76 - 17.92 + (2.101)0.284\sqrt{\tfrac{1}{10} + \tfrac{1}{10}}$$

$$-1.16 - 0.27 \leq \mu_1 - \mu_2 \leq -1.16 + 0.27$$

$$-1.43 \leq \mu_1 - \mu_2 \leq -0.89$$

Thus, the 95 percent confidence interval estimate on the difference in means extends from -1.43 kgf/cm^2 to -0.89 kgf/cm^2. Put another way, the confidence interval is $\mu_1 - \mu_2 = -1.16$ kgf/cm$^2 \pm 0.27$ kgf/cm^2, or the difference in mean strengths is -1.16 kgf/cm^2, and the accuracy of this estimate is ± 0.27 kgf/cm^2. Note that because $\mu_1 - \mu_2 = 0$ is *not* included in this interval, the data do not support the hypothesis that $\mu_1 = \mu_2$ at the 5 percent level of significance. It is likely that the mean strength of the unmodified formulation exceeds the mean strength of the modified formulation. Notice

from Table 2-2 that Minitab also reported this confidence interval when the hypothesis testing procedure was conducted.

2-4.4 The Case Where $\sigma_1^2 \neq \sigma_2^2$

If we are testing

$$H_0: \mu_1 = \mu_2$$
$$H_1: \mu_1 \neq \mu_2$$

and cannot reasonably assume that the variances σ_1^2 and σ_2^2 are equal, then the two-sample t-test must be modified slightly. The test statistic becomes

$$t_0 = \frac{\bar{y}_1 - \bar{y}_2}{\sqrt{\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}}} \tag{2-31}$$

This statistic is not distributed exactly as t. However, the distribution of t_0 is well-approximated by t if we use

$$v = \frac{\left(\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}\right)^2}{\frac{(S_1^2/n_1)^2}{n_1 - 1} + \frac{(S_2^2/n_2)^2}{n_2 - 1}} \tag{2-32}$$

as the degrees of freedom. A strong indication of unequal variances on a normal probability plot would be a situation calling for this version of the t-test. You should be able to develop an equation for finding that confidence interval on the difference in mean for the unequal variances case easily.

2-4.5 The Case Where σ_1^2 and σ_2^2 Are Known

If the variances of both populations are *known*, then the hypotheses

$$H_0: \mu_1 = \mu_2$$
$$H_1: \mu_1 \neq \mu_2$$

may be tested using the statistic

$$Z_0 = \frac{\bar{y}_1 - \bar{y}_2}{\sqrt{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}}} \tag{2-33}$$

If both populations are normal, or if the sample sizes are large enough so that the central limit theorem applies, the distribution of Z_0 is $N(0, 1)$ if the null hypothesis is true. Thus, the critical region would be found using the normal distribution rather than the t. Specifically, we would reject H_0 if $|Z_0| > Z_{\alpha/2}$, where $Z_{\alpha/2}$ is the upper $\alpha/2$ percentage point of the standard normal distribution.

Unlike the t-test of the previous sections, the test on means with known variances does not require the assumption of sampling from normal populations. One can use the central limit theorem to justify an approximate normal distribution for the difference in sample means $\bar{y}_1 - \bar{y}_2$.

The $100(1 - \alpha)$ percent confidence interval on $\mu_1 - \mu_2$ where the variances are known is

$$\bar{y}_1 - \bar{y}_2 - Z_{\alpha/2}\sqrt{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}} \leq \mu_1 - \mu_2 \leq \bar{y}_1 - \bar{y}_2 + Z_{\alpha/2}\sqrt{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}} \quad (2\text{-}34)$$

As noted previously, the confidence interval is often a useful supplement to the hypothesis testing procedure.

2-4.6 Comparing a Single Mean to a Specified Value

Some experiments involve comparing only one population mean μ to a specified value, say, μ_0. The hypotheses are

$$H_0: \mu = \mu_0$$
$$H_1: \mu \neq \mu_0$$

If the population is normal with known variance, or if the population is nonnormal but the sample size is large enough so that the central limit theorem applies, then the hypothesis may be tested using a direct application of the normal distribution. The test statistic is

$$Z_0 = \frac{\bar{y} - \mu_0}{\sigma/\sqrt{n}} \quad (2\text{-}35)$$

If $H_0: \mu = \mu_0$ is true, then the distribution of Z_0 is $N(0, 1)$. Therefore, the decision rule for $H_0: \mu = \mu_0$ is to reject the null hypothesis if $|Z_0| > Z_{\alpha/2}$. The value of the mean μ_0 specified in the null hypothesis is usually determined in one of three ways. It may result from past evidence, knowledge, or experimentation. It may be the result of some theory or model describing the situation under study. Finally, it may be the result of contractual specifications.

The $100(1 - \alpha)$ percent confidence interval on the true population mean is

$$\bar{y} - Z_{\alpha/2}\sigma/\sqrt{n} \leq \mu \leq \bar{y} + Z_{\alpha/2}\sigma/\sqrt{n} \quad (2\text{-}36)$$

EXAMPLE 2-1

A vendor submits lots of fabric to a textile manufacturer. The manufacturer wants to know if the lot average breaking strength exceeds 200 psi. If so, she wants to accept the lot. Past experience indicates that a reasonable value for the variance of breaking strength is $100(\text{psi})^2$. The hypotheses to be tested are

$$H_0: \mu = 200$$
$$H_1: \mu > 200$$

Note that this is a one-sided alternative hypothesis. Thus, we would accept the lot only if the null hypothesis $H_0: \mu = 200$ could be rejected (i.e., if $Z_0 > Z_\alpha$).

Four specimens are randomly selected, and the average breaking strength observed is $\bar{y} = 214$ psi. The value of the test statistic is

$$Z_0 = \frac{\bar{y} - \mu_0}{\sigma/\sqrt{n}} = \frac{214 - 200}{10/\sqrt{4}} = 2.80$$

If a type I error of $\alpha = 0.05$ is specified, we find $Z_\alpha = Z_{0.05} = 1.645$ from Appendix Table I. Thus H_0 is rejected, and we conclude that the lot average breaking strength exceeds 200 psi.

If the variance of the population is unknown, we must make the additional assumption that the population is normally distributed, although moderate departures from normality will not seriously affect the results.

To test $H_0: \mu = \mu_0$ in the variance unknown case, the sample variance S^2 is used to estimate σ^2. Replacing σ with S in Equation 2-35, we have the test statistic

$$t_0 = \frac{\bar{y} - \mu_0}{S/\sqrt{n}} \tag{2-37}$$

The null hypothesis $H_0: \mu = \mu_0$ would be rejected if $|t_0| > t_{\alpha/2,n-1}$, where $t_{\alpha/2,n-1}$ denotes the upper $\alpha/2$ percentage point of the t distribution with $n - 1$ degrees of freedom. The $100(1 - \alpha)$ percent confidence interval in this case is

$$\bar{y} - t_{\alpha/2,n-1}S/\sqrt{n} \leq \mu \leq \bar{y} + t_{\alpha/2,n-1}S/\sqrt{n} \tag{2-38}$$

2-4.7 Summary

Tables 2-3 and 2-4 summarize the test procedures discussed above for sample means. Critical regions are shown for both two-sided and one-sided alternative hypotheses.

Table 2-3 Tests on Means with Variance Known

Hypothesis	Test Statistic	Criteria for Rejection
$H_0: \mu = \mu_0$ $H_1: \mu \neq \mu_0$	$Z_0 = \dfrac{\bar{y} - \mu_0}{\sigma/\sqrt{n}}$	$\lvert Z_0 \rvert > Z_{\alpha/2}$
$H_0: \mu = \mu_0$ $H_1: \mu < \mu_0$		$Z_0 < -Z_\alpha$
$H_0: \mu = \mu_0$ $H_1: \mu > \mu_0$		$Z_0 > Z_\alpha$
$H_0: \mu_1 = \mu_2$ $H_1: \mu_1 \neq \mu_2$	$Z_0 = \dfrac{\bar{y}_1 - \bar{y}_2}{\sqrt{\dfrac{\sigma_1^2}{n_1} + \dfrac{\sigma_2^2}{n_2}}}$	$\lvert Z_0 \rvert > Z_{\alpha/2}$
$H_0: \mu_1 = \mu_2$ $H_1: \mu_1 < \mu_2$		$Z_0 < -Z_\alpha$
$H_0: \mu_1 = \mu_2$ $H_1: \mu_1 > \mu_2$		$Z_0 > Z_\alpha$

Table 2-4 Tests on Means of Normal Distributions, Variance Unknown

Hypothesis	Test Statistic	Criteria for Rejection
$H_0: \mu = \mu_0$ $H_1: \mu \neq \mu_0$	$t_0 = \dfrac{\bar{y} - \mu_0}{S/\sqrt{n}}$	$\lvert t_0 \rvert > t_{\alpha/2,n-1}$
$H_0: \mu = \mu_0$ $H_1: \mu < \mu_0$		$t_0 < -t_{\alpha,n-1}$
$H_0: \mu = \mu_0$ $H_1: \mu > \mu_0$		$t_0 > t_{\alpha,n-1}$
	if $\sigma_1^2 = \sigma_2^2$	
$H_0: \mu_1 = \mu_2$ $H_1: \mu_1 \neq \mu_2$	$t_0 = \dfrac{\bar{y}_1 - \bar{y}_2}{S_p\sqrt{\dfrac{1}{n_1} + \dfrac{1}{n_2}}}$ $v = n_1 + n_2 - 2$	$\lvert t_0 \rvert > t_{\alpha/2,v}$
	if $\sigma_1^2 \neq \sigma_2^2$	
$H_0: \mu_1 = \mu_2$ $H_1: \mu_1 < \mu_2$	$t_0 = \dfrac{\bar{y}_1 - \bar{y}_2}{\sqrt{\dfrac{S_1^2}{n_1} + \dfrac{S_2^2}{n_2}}}$	$t_0 < -t_{\alpha,v}$
$H_0: \mu_1 = \mu_2$ $H_1: \mu_1 > \mu_2$	$v = \dfrac{\left(\dfrac{S_1^2}{n_1} + \dfrac{S_2^2}{n_2}\right)^2}{\dfrac{(S_1^2/n_1)^2}{n_1 - 1} + \dfrac{(S_2^2/n_2)^2}{n_2 - 1}}$	$t_0 > t_{\alpha,v}$

2-5 INFERENCES ABOUT THE DIFFERENCES IN MEANS, PAIRED COMPARISON DESIGNS

2-5.1 The Paired Comparison Problem

In some simple comparative experiments we can greatly improve the precision by making comparisons within matched pairs of experimental material. For example, consider a hardness testing machine that presses a rod with a pointed tip into a metal specimen with a known force. By measuring the depth of the depression caused by the tip, the hardness of the specimen is determined. Two different tips are available for this machine, and although the precision (variability) of the measurements made by the two tips seems to be the same, it is suspected that one tip produces different hardness readings than the other.

An experiment could be performed as follows. A number of metal specimens (e.g., 20) could be randomly selected. Half of these specimens could be tested by tip 1 and the other half by tip 2. The exact assignment of specimens to tips would be randomly determined. Because this is a completely randomized design, the average hardness of the two samples could be compared using the t-test described in Section 2-4.

A little reflection will reveal a serious disadvantage in the completely randomized design for this problem. Suppose the metal specimens were cut from different bar stock

that were produced in different heats or that were not exactly homogeneous in some other way that might affect the hardness. This lack of homogeneity between specimens will contribute to the variability of the hardness measurements and will tend to inflate the experimental error, thus making a true difference between tips harder to detect.

To protect against this possibility, consider an alternative experimental design. Assume that each specimen is large enough so that *two* hardness determinations may be made on it. This alternative design would consist of dividing each specimen into two parts, then randomly assigning one tip to one-half of each specimen and the other tip to the remaining half. The order in which the tips are tested for a particular specimen would also be randomly selected. The experiment, when performed according to this design with 10 specimens, produced the (coded) data shown in Table 2-5.

We may write a **statistical model** that describes the data from this experiment as

$$y_{ij} = \mu_i + \beta_j + \epsilon_{ij} \begin{cases} i = 1, 2 \\ j = 1, 2, \ldots, 10 \end{cases} \tag{2-39}$$

where y_{ij} is the observation on hardness for tip i on specimen j, μ_i is the true mean hardness of the ith tip, β_j is an effect on hardness due to the jth specimen, and ε_{ij} is a random experimental error with mean zero and variance σ_i^2. That is, σ_1^2 is the variance of the hardness measurements from tip 1 and σ_2^2 is the variance of the hardness measurements from tip 2.

Note that if we compute the jth paired difference

$$d_j = y_{1j} - y_{2j} \qquad j = 1, 2, \ldots, 10 \tag{2-40}$$

the expected value of this difference is

$$\begin{aligned} \mu_d &= E(d_j) \\ &= E(y_{1j} - y_{2j}) \\ &= E(y_{1j}) - E(y_{2j}) \\ &= \mu_1 + \beta_j - (\mu_2 + \beta_j) \\ &= \mu_1 - \mu_2 \end{aligned}$$

That is, we may make inferences about the difference in the mean hardness readings of the two tips $\mu_1 - \mu_2$ by making inferences about the mean of the differences μ_d. Notice

Table 2-5 Data for the Hardness Testing Experiment

Specimen	Tip 1	Tip 2
1	7	6
2	3	3
3	3	5
4	4	3
5	8	8
6	3	2
7	2	4
8	9	9
9	5	4
10	4	5

that the additive effect of the specimens β_j cancels out when the observations are paired in this manner.

Testing $H_0: \mu_1 = \mu_2$ is equivalent to testing

$$H_0: \mu_d = 0$$
$$H_1: \mu_d \neq 0$$

The test statistic for this hypothesis is

$$t_0 = \frac{\bar{d}}{S_d/\sqrt{n}} \tag{2-41}$$

where

$$\bar{d} = \frac{1}{n}\sum_{j=1}^{n} d_j \tag{2-42}$$

is the sample mean of the differences and

$$S_d = \left[\frac{\sum_{j=1}^{n}(d_j - \bar{d})^2}{n-1}\right]^{1/2} = \left[\frac{\sum_{j=1}^{n} d_j^2 - \frac{1}{n}\left(\sum_{j=1}^{n} d_j\right)^2}{n-1}\right]^{1/2} \tag{2-43}$$

is the sample standard deviation of the differences. $H_0: \mu_d = 0$ would be rejected if $|t_0| > t_{\alpha/2,n-1}$. Because the observations from the factor levels are "paired" on each experimental unit, this procedure is usually called the **paired *t*-test**.

For the data in Table 2-5, we find

$$d_1 = 7 - 6 = 1 \qquad d_6 = 3 - 2 = 1$$
$$d_2 = 3 - 3 = 0 \qquad d_7 = 2 - 4 = -2$$
$$d_3 = 3 - 5 = -2 \qquad d_8 = 9 - 9 = 0$$
$$d_4 = 4 - 3 = 1 \qquad d_9 = 5 - 4 = 1$$
$$d_5 = 8 - 8 = 0 \qquad d_{10} = 4 - 5 = -1$$

Thus,

$$\bar{d} = \frac{1}{n}\sum_{j=1}^{n} d_j = \frac{1}{10}(-1) = -0.10$$

$$S_d = \left[\frac{\sum_{j=1}^{n} d_j^2 - \frac{1}{n}\left(\sum_{j=1}^{n} d_j\right)^2}{n-1}\right]^{1/2} = \left[\frac{13 - \frac{1}{10}(-1)^2}{10-1}\right]^{1/2} = 1.20$$

Suppose we choose $\alpha = 0.05$. Now to make a decision, we would compute t_0 and reject H_0 if $|t_0| > t_{0.025,9} = 2.262$.

The computed value of the paired t-test statistic is

$$t_0 = \frac{\bar{d}}{S_d/\sqrt{n}}$$
$$= \frac{-0.10}{1.20/\sqrt{10}}$$
$$= -0.26$$

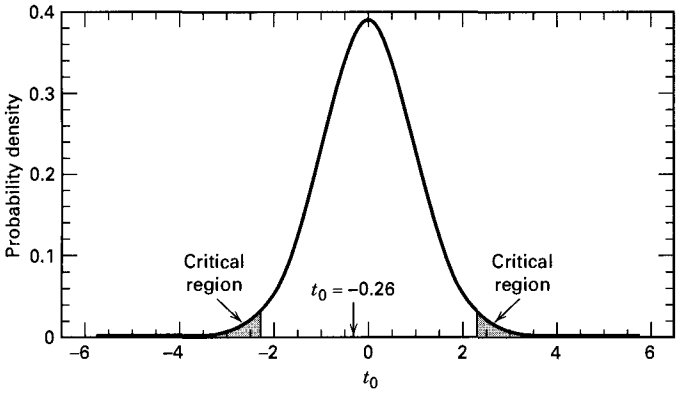


Figure 2-13 The reference distribution (t with 9 degrees of freedom) for the hardness testing problem.

and because $|t_0| = 0.26 \not> t_{0.025,9} = 2.262$, we cannot reject the hypothesis $H_0: \mu_d = 0$. That is, there is no evidence to indicate that the two tips produce different hardness readings. Figure 2-13 shows the t_0 distribution with 9 degrees of freedom, the reference distribution for this test, with the value of t_0 shown relative to the critical region.

Table 2-6 shows the computer output from the Minitab paired t-test procedure for this problem. Notice that the P-value for this test is $P \simeq 0.80$, implying that we cannot reject the null hypothesis at *any* reasonable level of significance.

2-5.2 Advantages of the Paired Comparison Design

The design actually used for this experiment is called the **paired comparison design**, and it illustrates the blocking principle discussed in Section 1-3. Actually, it is a special case of a more general type of design called the **randomized block design**. The term *block* refers to a relatively homogeneous experimental unit (in our case, the metal specimens are the blocks), and the block represents a restriction on complete randomization because the treatment combinations are only randomized within the block. We look at designs of this type in Chapter 4. In that chapter the mathematical model for the design, Equation 2-39, is written in a slightly different form.

Table 2-6 Minitab Paired t-Test Results for the Hardness Testing Example

Paired t-Test and Confidence Interval

```
Paired T for Tip 1 - Tip 2

                N        Mean       StDev     SE Mean
Tip 1          10       4.800       2.394       0.757
Tip 2          10       4.900       2.234       0.706
Difference     10      -0.100       1.197       0.379

95% CI for mean difference: (-0.956, 0.756)
t-Test of mean difference = 0 (vs not = 0):
T-Value = -0.26  P-Value = 0.798
```

Before leaving this experiment, several points should be made. Note that, although $2n = 2(10) = 20$ observations have been taken, only $n - 1 = 9$ degrees of freedom are available for the t statistic. (We know that as the degrees of freedom for t increase the test becomes more sensitive.) By blocking or pairing, we have effectively "lost" $n - 1$ degrees of freedom, but we hope we have gained a better knowledge of the situation by eliminating an additional source of variability (the difference between specimens). We may obtain an indication of the quality of information produced from the paired design by comparing the standard deviation of the differences S_d with the pooled standard deviation S_p that would have resulted had the experiment been conducted in a completely randomized manner and the data of Table 2-5 been obtained. Using the data in Table 2-5 as two independent samples, we compute the pooled standard deviation from Equation 2-25 to be $S_p = 2.32$. Comparing this value to $S_d = 1.20$, we see that blocking or pairing has reduced the estimate of variability by nearly 50 percent. We may also express this information in terms of a confidence interval on $\mu_1 - \mu_2$. Using the paired data, a 95 percent confidence interval on $\mu_1 - \mu_2$ is

$$\bar{d} \pm t_{0.025,9} S_d/\sqrt{n}$$

$$-0.10 \pm (2.262)(1.20)/\sqrt{10}$$

$$-0.10 \pm 0.86$$

Conversely, using the pooled or independent analysis, a 95 percent confidence interval on $\mu_1 - \mu_2$ is

$$\bar{y}_1 - \bar{y}_2 \pm t_{0.025,18} S_p \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}$$

$$4.80 - 4.90 \pm (2.101)(2.32)\sqrt{\tfrac{1}{10} + \tfrac{1}{10}}$$

$$-0.10 \pm 2.18$$

The confidence interval based on the paired analysis is much narrower than the confidence interval from the independent analysis. This illustrates the **noise reduction** property of blocking.

Blocking is not always the best design strategy. If the within-block variability is the same as the between-block variability, the variance of $\bar{y}_1 - \bar{y}_2$ will be the same regardless of which design is used. Actually, blocking in this situation would be a poor choice of design because blocking results in the loss of $n - 1$ degrees of freedom and will actually lead to a wider confidence interval on $\mu_1 - \mu_2$. A further discussion of blocking is given in Chapter 4.

2-6 INFERENCES ABOUT THE VARIANCES OF NORMAL DISTRIBUTIONS

In many experiments, we are interested in possible differences in the mean response for two treatments. However, in some experiments it is the comparison of variability in the data that is important. In the food and beverage industry, for example, it is important that the variability of filling equipment be small so that all packages have close to the nominal net weight or volume of content. In chemical laboratories, we may wish to

compare the variability of two analytical methods. We now briefly examine tests of hypotheses and confidence intervals for variances of normal distributions. Unlike the tests on means, the procedures for tests on variances are rather sensitive to the normality assumption. A good discussion of the normality assumption is in Appendix 2A of Davies (1956).

Suppose we wish to test the hypothesis that the variance of a normal population equals a constant, for example, σ_0^2. Stated formally, we wish to test

$$\begin{aligned} H_0&: \sigma^2 = \sigma_0^2 \\ H_1&: \sigma^2 \neq \sigma_0^2 \end{aligned} \tag{2-44}$$

The test statistic for Equation 2-44 is

$$\chi_0^2 = \frac{SS}{\sigma_0^2} = \frac{(n-1)S^2}{\sigma_0^2} \tag{2-45}$$

where $SS = \Sigma_{i=1}^{n}(y_i - y)^2$ is the corrected sum of squares of the sample observations. The appropriate reference distribution for χ_0^2 is the chi-square distribution with $n - 1$ degrees of freedom. The null hypothesis is rejected if $\chi_0^2 > \chi_{\alpha/2,n-1}^2$ or if $\chi_0^2 < \chi_{1-(\alpha/2),n-1}^2$, where $\chi_{\alpha/2,n-1}^2$ and $\chi_{1-(\alpha/2),n-1}^2$ are the upper $\alpha/2$ and lower $1 - (\alpha/2)$ percentage points of the chi-square distribution with $n - 1$ degrees of freedom, respectively. Table 2-7 (on the facing page) gives the critical regions for the one-sided alternative hypotheses. The $100(1 - \alpha)$ percent confidence interval on σ^2 is

$$\frac{(n-1)S^2}{\chi_{\alpha/2,n-1}^2} \leqslant \sigma^2 \leqslant \frac{(n-1)S^2}{\chi_{1-(\alpha/2),n-1}^2} \tag{2-46}$$

Now consider testing the equality of the variances of two normal populations. If independent random samples of size n_1 and n_2 are taken from populations 1 and 2, respectively, the test statistic for

$$\begin{aligned} H_0&: \sigma_1^2 = \sigma_2^2 \\ H_1&: \sigma_1^2 \neq \sigma_2^2 \end{aligned} \tag{2-47}$$

is the ratio of the sample variances

$$F_0 = \frac{S_1^2}{S_2^2} \tag{2-48}$$

The appropriate reference distribution for F_0 is the F distribution with $n_1 - 1$ numerator degrees of freedom and $n_2 - 1$ denominator degrees of freedom. The null hypothesis would be rejected if $F_0 > F_{\alpha/2,n_1-1,n_2-1}$ or if $F_0 < F_{1-(\alpha/2),n_1-1,n_2-1}$, where $F_{\alpha/2,n_1-1,n_2-1}$ and $F_{1-(\alpha/2),n_1-1,n_2-1}$ denote the upper $\alpha/2$ and lower $1 - (\alpha/2)$ percentage points of the F distribution with $n_1 - 1$ and $n_2 - 1$ degrees of freedom. Table IV of the Appendix gives only upper-tail percentage poins of F; however, the upper- and lower-tail points are related by

$$F_{1-\alpha,v_1,v_2} = \frac{1}{F_{\alpha,v_2,v_1}} \tag{2-49}$$

Table 2-7 Tests on Variances of Normal Distributions

Hypothesis	Test Statistic	Criteria for Rejection
$H_0: \sigma^2 = \sigma_0^2$ $H_1: \sigma^2 \neq \sigma_0^2$	$\chi_0^2 = \dfrac{(n-1)S^2}{\sigma_0^2}$	$\chi_0^2 > \chi^2_{\alpha/2,n-1}$ or $\chi_0^2 < \chi^2_{1-\alpha/2,n-1}$
$H_0: \sigma^2 = \sigma_0^2$ $H_1: \sigma^2 < \sigma_0^2$		$\chi_0^2 < \chi^2_{1-\alpha,n-1}$
$H_0: \sigma^2 = \sigma_0^2$ $H_1: \sigma^2 > \sigma_0^2$		$\chi_0^2 > \chi^2_{\alpha,n-1}$
$H_0: \sigma_1^2 = \sigma_2^2$ $H_1: \sigma_1^2 \neq \sigma_2^2$	$F_0 = \dfrac{S_1^2}{S_2^2}$	$F_0 > F_{\alpha/2,n_1-1,n_2-1}$ or $F_0 < F_{1-\alpha/2,n_1-1,n_2-1}$
$H_0: \sigma_1^2 = \sigma_2^2$ $H_1: \sigma_1^2 < \sigma_2^2$	$F_0 = \dfrac{S_2^2}{S_1^2}$	$F_0 > F_{\alpha,n_2-1,n_1-1}$
$H_0: \sigma_1^2 = \sigma_2^2$ $H_1: \sigma_1^2 > \sigma_2^2$	$F_0 = \dfrac{S_1^2}{S_2^2}$	$F_0 > F_{\alpha,n_1-1,n_2-1}$

Test procedures for more than two variances are discussed in Chapter 3, Section 3-4.3. We will also discuss the use of the variance or standard deviation as a response variable in more general experimental settings.

EXAMPLE 2-2

A chemical engineer is investigating the inherent variability of two types of test equipment that can be used to monitor the output of a production process. He suspects that the old equipment, type 1, has a larger variance than the new one. Thus, he wishes to test the hypothesis

$$H_0: \sigma_1^2 = \sigma_2^2$$
$$H_1: \sigma_1^2 > \sigma_2^2$$

Two random samples of $n_1 = 12$ and $n_2 = 10$ observations are taken, and the sample variances are $S_1^2 = 14.5$ and $S_2^2 = 10.8$. The test statistic is

$$F_0 = \frac{S_1^2}{S_2^2} = \frac{14.5}{10.8} = 1.34$$

From Appendix Table IV we find that $F_{0.05,11,9} = 3.10$, so the null hypothesis cannot be rejected. That is, we have found insufficient statistical evidence to conclude that the variance of the old equipment is greater than the variance of the new equipment.

The $100(1 - \alpha)$ confidence interval for the ratio of the population variances σ_1^2/σ_2^2 is

$$\frac{S_1^2}{S_2^2} F_{1-\alpha/2,n_2-1,n_1-1} \leq \frac{\sigma_1^2}{\sigma_2^2} \leq \frac{S_1^2}{S_2^2} F_{\alpha/2,n_2-1,n_1-1} \tag{2-50}$$

To illustrate the use of Equation 2-50, the 95 percent confidence interval for the ratio of variances σ_1^2/σ_2^2 in Example 2-2 is, using $F_{0.025,9,11} = 3.59$ and $F_{0.975,9,11} = 1/F_{0.025,11,9} = 1/3.92 = 0.255$,

$$\frac{14.5}{10.8}(0.255) \leq \frac{\sigma_1^2}{\sigma_2^2} \leq \frac{14.5}{10.8}(3.59)$$

$$0.34 \leq \frac{\sigma_1^2}{\sigma_2^2} \leq 4.81$$

2-7 PROBLEMS

2-1. The breaking strength of a fiber is required to be at least 150 psi. Past experience has indicated that the standard deviation of breaking strength is $\sigma = 3$ psi. A random sample of four specimens is tested, and the results are $y_1 = 145$, $y_2 = 153$, $y_3 = 150$, and $y_4 = 147$.
(a) State the hypotheses that you think should be tested in this experiment.
(b) Test these hypotheses using $\alpha = 0.05$. What are your conclusions?
(c) Find the P-value for the test in part (b).
(d) Construct a 95 percent confidence interval on the mean breaking strength.

2-2. The viscosity of a liquid detergent is supposed to average 800 centistokes at 25°C. A random sample of 16 batches of detergent is collected, and the average viscosity is 812. Suppose we know that the standard deviation of viscosity is $\sigma = 25$ centistokes.
(a) State the hypotheses that should be tested.
(b) Test these hypotheses using $\alpha = 0.05$. What are your conclusions?
(c) What is the P-value for the test?
(d) Find a 95 percent confidence interval on the mean.

2-3. The diameters of steel shafts produced by a certain manufacturing process should have a mean diameter of 0.255 inches. The diameter is known to have a standard deviation of $\sigma = 0.0001$ inch. A random sample of 10 shafts has an average diameter of 0.2545 inch.
(a) Set up appropriate hypotheses on the mean μ.
(b) Test these hypotheses using $\alpha = 0.05$. What are your conclusions?
(c) Find the P-value for this test.
(d) Construct a 95 percent confidence interval on the mean shaft diameter.

2-4. A normally distributed random variable has an unknown mean μ and a known variance $\sigma^2 = 9$. Find the sample size required to construct a 95 percent confidence interval on the mean that has total width of 1.0.

2-5. The shelf life of a carbonated beverage is of interest. Ten bottles are randomly selected and tested, and the following results are obtained:

Days	
108	138
124	163
124	159
106	134
115	139

(a) We would like to demonstrate that the mean shelf life exceeds 120 days. Set up appropriate hypotheses for investigating this claim.
(b) Test these hypotheses using $\alpha = 0.01$. What are your conclusions?

(c) Find the P-value for the test in part (b).
(d) Construct a 99 percent confidence interval on the mean shelf life.

2-6. Consider the shelf life data in Problem 2-5. Can shelf life be described or modeled adequately by a normal distribution? What effect would violation of this assumption have on the test procedure you used in solving Problem 2-5?

2-7. The time to repair an electronic instrument is a normally distributed random variable measured in hours. The repair times for 16 such instruments chosen at random are as follows:

Hours			
159	280	101	212
224	379	179	264
222	362	168	250
149	260	485	170

(a) You wish to know if the mean repair time exceeds 225 hours. Set up appropriate hypotheses for investigating this issue.
(b) Test the hypotheses you formulated in part (a). What are your conclusions? Use $\alpha = 0.05$.
(c) Find the P-value for the test.
(d) Construct a 95 percent confidence interval on mean repair time.

2-8. Reconsider the repair time data in Problem 2-7. Can repair time, in your opinion, be adequately modeled by a normal distribution?

2-9. Two machines are used for filling plastic bottles with a net volume of 16.0 ounces. The filling processes can be assumed to be normal, with standard deviations of $\sigma_1 = 0.015$ and $\sigma_2 = 0.018$. The quality engineering department suspects that both machines fill to the same net volume, whether or not this volume is 16.0 ounces. An experiment is performed by taking a random sample from the output of each machine.

Machine 1		Machine 2	
16.03	16.01	16.02	16.03
16.04	15.96	15.97	16.04
16.05	15.98	15.96	16.02
16.05	16.02	16.01	16.01
16.02	15.99	15.99	16.00

(a) State the hypotheses that should be tested in this experiment.
(b) Test these hypotheses using $\alpha = 0.05$. What are your conclusions?
(c) Find the P-value for this test.
(d) Find a 95 percent confidence interval on the difference in mean fill volume for the two machines.

2-10. Two types of plastic are suitable for use by an electronic calculator manufacturer. The breaking strength of this plastic is important. It is known that $\sigma_1 = \sigma_2 = 1.0$ psi. From random samples of $n_1 = 10$ and $n_2 = 12$ we obtain $\bar{y}_1 = 162.5$ and $\bar{y}_2 = 155.0$. The company will not adopt plastic 1 unless its breaking strength exceeds that of plastic 2 by at least 10 psi. Based on the sample information, should they use plastic 1? In answering this question, set up and test appropriate hypotheses using $\alpha = 0.01$. Construct a 99 percent confidence interval on the true mean difference in breaking strength.

2-11. The following are the burning times of chemical flares of two different formulations. The design engineers are interested in both the mean and variance of the burning times.

Type 1		Type 2	
65	82	64	56
81	67	71	69
57	59	83	74
66	75	59	82
82	70	65	79

(a) Test the hypothesis that the two variances are equal. Use $\alpha = 0.05$.
(b) Using the results of (a), test the hypothesis that the mean burning times are equal. Use $\alpha = 0.05$. What is the P-value for this test?
(c) Discuss the role of the normality assumption in this problem. Check the assumption of normality for both types of flares.

2-12. An article in *Solid State Technology*, "Orthogonal Design for Process Optimization and Its Application to Plasma Etching" by G. Z. Yin and D. W. Jillie (May, 1987) describes an experiment to determine the effect of the C_2F_6 flow rate on the uniformity of the etch on a silicon wafer used in integrated circuit manufacturing. Data for two flow rates are as follows:

C_2F_6 Flow (SCCM)	Uniformity Observation					
	1	2	3	4	5	6
125	2.7	4.6	2.6	3.0	3.2	3.8
200	4.6	3.4	2.9	3.5	4.1	5.1

(a) Does the C_2F_6 flow rate affect average etch uniformity? Use $\alpha = 0.05$.
(b) What is the P-value for the test in part (a)?
(c) Does the C_2F_6 flow rate affect the wafer-to-wafer variability in etch uniformity? Use $\alpha = 0.05$.
(d) Draw box plots to assist in the interpretation of the data from this experiment.

2-13. A new filtering device is installed in a chemical unit. Before its installation, a random sample yielded the following information about the percentage of impurity: $\bar{y}_1 = 12.5$, $S_1^2 = 101.17$, and $n_1 = 8$. After installation, a random sample yielded $\bar{y}_2 = 10.2$, $S_2^2 = 94.73$, $n_2 = 9$.
(a) Can you conclude that the two variances are equal? Use $\alpha = 0.05$.
(b) Has the filtering device reduced the percentage of impurity significantly? Use $\alpha = 0.05$.

2-14. Twenty observations on etch uniformity on silicon wafers are taken during a qualification experiment for a plasma etcher. The data are as follows:

5.34	6.65	4.76	5.98	7.25
6.00	7.55	5.54	5.62	6.21
5.97	7.35	5.44	4.39	4.98
5.25	6.35	4.61	6.00	5.32

(a) Construct a 95 percent confidence interval estimate of σ^2.
(b) Test the hypothesis that $\sigma^2 = 1.0$. Use $\alpha = 0.05$. What are your conclusions?

(c) Discuss the normality assumption and its role in this problem.
(d) Check normality by constructing a normal probability plot. What are your conclusions?

2-15. The diameter of a ball bearing was measured by 12 inspectors, each using two different kinds of calipers. The results were

Inspector	Caliper 1	Caliper 2
1	0.265	0.264
2	0.265	0.265
3	0.266	0.264
4	0.267	0.266
5	0.267	0.267
6	0.265	0.268
7	0.267	0.264
8	0.267	0.265
9	0.265	0.265
10	0.268	0.267
11	0.268	0.268
12	0.265	0.269

(a) Is there a significant difference between the means of the population of measurements from which the two samples were selected? Use $\alpha = 0.05$.
(b) Find the P-value for the test in part (a).
(c) Construct a 95 percent confidence interval on the difference in mean diameter measurements for the two types of calipers.

2-16. An article in the *Journal of Strain Analysis* (vol. 18, no. 2, 1983) compares several procedures for predicting the shear strength for steel plate girders. Data for nine girders in the form of the ratio of predicted to observed load for two of these procedures, the Karlsruhe and Lehigh methods, are as follows:

Girder	Karlsruhe Method	Lehigh Method
S1/1	1.186	1.061
S2/1	1.151	0.992
S3/1	1.322	1.063
S4/1	1.339	1.062
S5/1	1.200	1.065
S2/1	1.402	1.178
S2/2	1.365	1.037
S2/3	1.537	1.086
S2/4	1.559	1.052

(a) Is there any evidence to support a claim that there is a difference in mean performance between the two methods? Use $\alpha = 0.05$.
(b) What is the P-value for the test in part (a)?
(c) Construct a 95 percent confidence interval for the difference in mean predicted to observed load.
(d) Investigate the normality assumption for both samples.
(e) Investigate the normality assumption for the difference in ratios for the two methods.
(f) Discuss the role of the normality assumption in the paired t-test.

2-17. The deflection temperature under load for two different formulations of ABS plastic pipe is being studied. Two samples of 12 observations each are prepared using each formulation and the deflection temperatures (in °F) are reported below:

Formulation 1			Formulation 2		
206	193	192	177	176	198
188	207	210	197	185	188
205	185	194	206	200	189
187	189	178	201	197	203

(a) Construct normal probability plots for both samples. Do these plots support assumptions of normality and equal variance for both samples?
(b) Does the data support the claim that the mean deflection temperature under load for formulation 1 exceeds that of formulation 2? Use $\alpha = 0.05$.
(c) What is the P-value for the test in part (a)?

2-18. Refer to the data in Problem 2-17. Do the data support a claim that the mean deflection temperature under load for formulation 1 exceeds that of formulation 2 by at least 3°F?

2-19. In semiconductor manufacturing wet chemical etching is often used to remove silicon from the backs of wafers prior to metalization. The etch rate is an important characteristic of this process. Two different etching solutions are being evaluated. Eight randomly selected wafers have been etched in each solution and the observed etch rates (in mils/min) are shown below.

Solution 1		Solution 2	
9.9	10.6	10.2	10.6
9.4	10.3	10.0	10.2
10.0	9.3	10.7	10.4
10.3	9.8	10.5	10.3

(a) Do the data indicate that the claim that both solutions have the same mean etch rate is valid? Use $\alpha = 0.05$ and assume equal variances.
(b) Find a 95 percent confidence interval on the difference in mean etch rates.
(c) Use normal probability plots to investigate the adequacy of the assumptions of normality and equal variances.

2-20. Two popular pain medications are being compared on the basis of the speed of absorption by the body. Specifically, tablet 1 is claimed to be absorbed twice as fast as tablet 2. Assume that σ_1^2 and σ_2^2 are known. Develop a test statistic for

$$H_0: 2\mu_1 = \mu_2$$
$$H_1: 2\mu_1 \neq \mu_2$$

2-21. Suppose we are testing

$$H_0: \mu_1 = \mu_2$$
$$H_1: \mu_1 \neq \mu_2$$

where σ_1^2 and σ_2^2 are known. Our sampling resources are constrained such that $n_1 + n_2 = N$. How should we allocate the N observations between the two populations to obtain the most powerful test?

2-22. Develop Equation 2-46 for a $100(1 - \alpha)$ percent confidence interval for the variance of a normal distribution.

2-23. Develop Equation 2-50 for a $100(1 - \alpha)$ percent confidence interval for the ratio σ_1^2/σ_2^2, where σ_1^2 and σ_2^2 are the variances of two normal distributions.

2-24. Develop an equation for finding a $100(1 - \alpha)$ percent confidence interval on the difference in the means of two normal distributions where $\sigma_1^2 \neq \sigma_2^2$. Apply your equation to the portland cement experiment data, and find a 95 pecent confidence interval.

2-25. Construct a data set for which the paired t-test statistic is very large, but for which the usual two-sample or pooled t-test statistic is small. In general, describe how you created the data. Does this give you any insight regarding how the paired t-test works?

3 Experiments with a Single Factor: The Analysis of Variance

In Chapter 2 we discussed methods for comparing two conditions or treatments. For example, the portland cement tension bond experiment involved two different mortar formulations. Another way to describe this experiment is as a single-factor experiment with two levels of the factor, where the factor is mortar formulation and the two levels are the two different formulation methods. Many experiments of this type involve more than two levels of the factor. In this chapter we present methods for the design and analysis of single-factor experiments with a levels of the factor (or a treatments). We will assume that the experiment has been completely randomized.

3-1 AN EXAMPLE

A product development engineer is interested in investigating the tensile strength of a new synthetic fiber that will be used to make cloth for men's shirts. The engineer knows from previous experience that the strength is affected by the weight percent of cotton used in the blend of materials for the fiber. Furthermore, she suspects that increasing the cotton content will increase the strength, at least initially. She also knows that cotton content should range between about 10 and 40 percent if the final product is to have other quality characteristics that are desired (such as the ability to take a permanent-press finishing treatment). The engineer decides to test specimens at five levels of cotton weight percent: 15, 20, 25, 30, and 35 percent. She also decides to test five specimens at each level of cotton content.

This is an example of a single-factor experiment with $a = 5$ **levels** of the factor and $n = 5$ **replicates**. The 25 runs should be made in random order. To illustrate how the run order may be randomized, suppose that we number the runs as follows:

Cotton Weight Percentage	Experimental Run Number				
15	1	2	3	4	5
20	6	7	8	9	10
25	11	12	13	14	15
30	16	17	18	19	20
35	21	22	23	24	25

Now we select a random number between 1 and 25. Suppose this number is 8. Then the number 8 observation (20 percent cotton) is run first. This process would be repeated until all 25 observations have been assigned a position in the test sequence.[1] Many computer software packages for assisting experimenters in selecting and constructing a design randomize the run order by using random numbers in this fashion.

Suppose that the test sequence obtained is

Test Sequence	Run Number	Cotton Weight Percentage
1	8	20
2	18	30
3	10	20
4	23	35
5	17	30
6	5	15
7	14	25
8	6	20
9	15	25
10	20	30
11	9	20
12	4	15
13	12	25
14	7	20
15	1	15
16	24	35
17	21	35
18	11	25
19	2	15
20	13	25
21	22	35
22	16	30
23	25	35
24	19	30
25	3	15

This randomized test sequence is necessary to prevent the effects of unknown nuisance variables, perhaps varying out of control during the experiment, from contaminating the

[1] The only restriction on randomization here is that if the same number (e.g., 8) is drawn again, it is discarded. This is a minor restriction and is ignored.

Table 3-1 Data (in lb/in^2) from the Tensile Strength Experiment

Cotton Weight Percentage	Observations					Total	Average
	1	2	3	4	5		
15	7	7	15	11	9	49	9.8
20	12	17	12	18	18	77	15.4
25	14	18	18	19	19	88	17.6
30	19	25	22	19	23	108	21.6
35	7	10	11	15	11	54	10.8
						376	15.04

results. To illustrate, suppose that we were to run the 25 test specimens in the original nonrandomized order (that is, all five 15 percent cotton specimens are tested first, all five 20 percent cotton specimens are tested next, and so on). If the tensile strength testing machine exhibits a warm-up effect such that the longer it is on, the lower the observed tensile strength readings will be, the warm-up effect will potentially contaminate the tensile strength data and destroy the validity of the experiment.

Suppose that the engineer runs the test in the random order we have determined. The observations that she obtains on tensile strength are shown in Table 3-1.

It is always a good idea to examine experimental data **graphically**. Figure 3-1 presents **box plots** for tensile strength at each level of cotton weight percent, and Figure 3-2 (on the facing page) is a **scatter diagram** of tensile strength versus cotton weight percentage. In Figure 3-2, the solid dots are the individual observations and the open circles are the average observed tensile strengths. Both graphs indicate that tensile strength increases as cotton content increases, up to about 30 percent cotton. Beyond 30 percent cotton, there is a marked decrease in tensile strength. There is no strong evidence to suggest that the variability in tensile strength around the average depends on the cotton weight percentage. Based on this simple graphical analysis, we strongly suspect that (1) cotton content affects tensile strength and (2) around 30 percent cotton results in maximum strength.

Suppose that we wish to be more **objective** in our analysis of the data. Specifically,

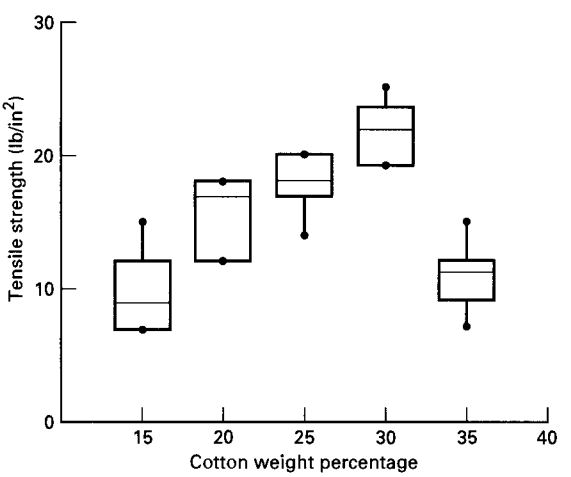


Figure 3-1 Box plots of tensile strength versus cotton weight percentage.

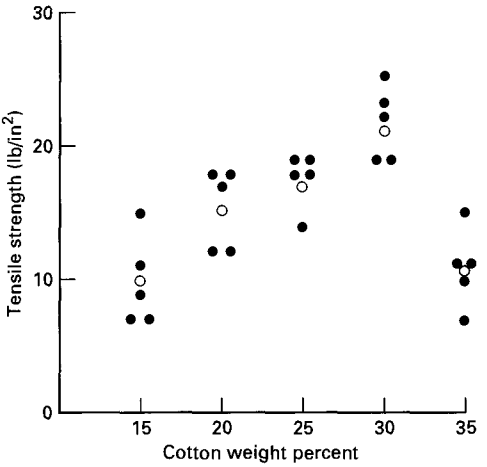


Figure 3-2 Scatter diagram of tensile strength versus cotton weight percentage.

suppose that we wish to test for differences between the mean strengths at all $a = 5$ levels of cotton weight percentage. Thus, we are interested in testing the equality of all five means. It might seem that this problem could be solved by performing a t-test for all the possible pairs of means. However, this is not the best solution to this problem because it would lead to considerable distortion in the type I error. For example, suppose we wish to test the equality of the five means using pairwise comparisons. There are 10 possible pairs, and if the probability of correctly accepting the null hypothesis for each individual test is $1 - \alpha = .95$, the probability of correctly accepting the null hypothesis for all 10 tests is $(.95)^{10} = .60$ if the tests are independent. Thus, a substantial increase in the type I error has occurred.

The appropriate procedure for testing the equality of several means is the **analysis of variance**. However, the analysis of variance has a much wider application than the problem above. It is probably the most useful technique in the field of statistical inference.

3-2 THE ANALYSIS OF VARIANCE

Suppose we have a **treatments** or different **levels** of a **single factor** that we wish to compare. The observed response from each of the a treatments is a random variable. The data would appear as in Table 3-2. An entry in Table 3-2 (e.g., y_{ij}) represents the jth observation taken under factor level or treatment i. There will be, in general, n obser-

Table 3-2 Typical Data for a Single-Factor Experiment

Treatment (level)	Observations				Totals	Averages
1	y_{11}	y_{12}	$\cdots$	y_{1n}	$y_{1.}$	$\bar{y}_{1.}$
2	y_{21}	y_{22}	$\cdots$	y_{2n}	$y_{2.}$	$\bar{y}_{2.}$
$\vdots$	$\vdots$	$\vdots$	$\cdots$	$\vdots$	$\vdots$	$\vdots$
a	y_{a1}	y_{a2}	$\cdots$	y_{an}	$y_{a.}$	$\bar{y}_{a.}$
					$y_{..}$	$\bar{y}_{..}$

vations under the ith treatment. Notice that Table 3-2 is the general case of the data from the tensile strength experiment in Table 3-1.

Models for the Data

We will find it useful to describe the observations from an experiment with a model. One way to write this model is

$$y_{ij} = \mu_i + \epsilon_{ij} \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, n \end{cases} \tag{3-1}$$

where y_{ij} is the ijth observation, μ_i is the mean of the ith factor level or treatment, and ϵ_{ij} is a **random error** component that incorporates all other sources of variability in the experiment including measurement, variability arising from uncontrolled factors, differences between the experimental units (such as test material, etc.) to which the treatments are applied, and the general background noise in the process (such as variability over time, effects of environmental variables, and so forth). It is convenient to think of the errors as having mean zero, so that $E(y_{ij}) = \mu_i$.

Equation 3-1 is called the **means model**. An alternative way to write a model for the data is to define

$$\mu_i = \mu + \tau_i, \qquad i = 1, 2, \ldots, a$$

so that Equation 3-1 becomes

$$y_{ij} = \mu + \tau_i + \epsilon_{ij} \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, n \end{cases} \tag{3-2}$$

In this form of the model, μ is a parameter common to all treatments called the **overall mean**, and τ_i is a parameter unique to the ith treatment called the ***i*th treatment effect**. Equation 3-2 is usually called the **effects model**.

Both the means model and the effects model are **linear statistical models**; that is, the response variable y_{ij} is a linear function of the model parameters. Although both forms of the model are useful, the effects model is more widely encountered in the experimental design literature. It has some intuitive appeal in that μ is a constant and the treatment effects τ_i represent deviations from this constant when the specific treatments are applied.

Equation 3-2 (or 3-1) is also called the **one-way** or **single-factor analysis of variance** model because only one factor is investigated. Furthermore, we will require that the experiment be performed in random order so that the environment in which the treatments are applied (often called the **experimental units**) is as uniform as possible. Thus, the experimental design is a **completely randomized design**. Our objectives will be to test appropriate hypotheses about the treatment means and to estimate them. For hypothesis testing, the model errors are assumed to be normally and independently distributed random variables with mean zero and variance σ^2. The variance σ^2 is assumed to be constant for all levels of the factor. This implies that the observations

$$y_{ij} \sim N(\mu + \tau_i, \sigma^2)$$

and that the observations are mutually independent.

Fixed or Random Factor?

The statistical model, Equation 3-2, describes two different situations with respect to the treatment effects. First, the a treatments could have been specifically chosen by the experimenter. In this situation we wish to test hypotheses about the treatment means, and our conclusions will apply only to the factor levels considered in the analysis. The conclusions cannot be extended to similar treatments that were not explicitly considered. We may also wish to estimate the model parameters (μ, τ_i, σ^2). This is called the **fixed effects model**. Alternatively, the a treatments could be a **random sample** from a larger population of treatments. In this situation we should like to be able to extend the conclusions (which are based on the sample of treatments) to all treatments in the population, whether they were explicitly considered in the analysis or not. Here the τ_i are random variables, and knowledge about the particular ones investigated is relatively useless. Instead, we test hypotheses about the variability of the τ_i and try to estimate this variability. This is called the **random effects model** or **components of variance model**. We will defer discussion of experiments with random factors to Chapter 12.

3-3 ANALYSIS OF THE FIXED EFFECTS MODEL

In this section, we develop the single-factor analysis of variance for the fixed effects model. Recall that $y_{i.}$ represents the total of the observations under the ith treatment. Let $\bar{y}_{i.}$ represent the average of the observations under the ith treatment. Similarly, let $y_{..}$ represent the grand total of all the observations and $\bar{y}_{..}$ represent the grand average of all the observations. Expressed symbolically,

$$\begin{aligned} y_{i.} &= \sum_{j=1}^{n} y_{ij}, \qquad \bar{y}_{i.} = y_{i.}/n \qquad i = 1, 2, \ldots, a \\ y_{..} &= \sum_{i=1}^{a} \sum_{j=1}^{n} y_{ij} \qquad \bar{y}_{..} = y_{..}/N \end{aligned} \tag{3-3}$$

where $N = an$ is the total number of observations. We see that the "dot" subscript notation implies summation over the subscript that it replaces.

We are interested in testing the equality of the a treatment means; that is, $E(y_{ij}) = \mu + \tau_i = \mu_i$, $i = 1, 2, \ldots, a$. The appropriate hypotheses are

$$\begin{aligned} H_0&: \mu_1 = \mu_2 = \cdots = \mu_a \\ H_1&: \mu_i \neq \mu_j \qquad \text{for at least one pair } (i, j) \end{aligned}$$

In the effects model, we break the ith treatment mean μ_i up into two components such that $\mu_i = \mu + \tau_i$. We usually think of μ as an overall mean so that

$$\frac{\sum_{i=1}^{a} \mu_i}{a} = \mu$$

This definition implies that

$$\sum_{i=1}^{a} \tau_i = 0$$

That is, the treatment or factor effects can be thought of as deviations from the overall mean.[2] Consequently, an equivalent way to write the above hypotheses is in terms of the treatment effects τ_i, say

$$H_0: \tau_1 = \tau_2 = \cdots \tau_a = 0$$
$$H_1: \tau_i \neq 0 \qquad \text{for at least one } i$$

Thus, we speak of testing the equality of treatment means or testing that the treatment effects (the τ_i) are zero. The appropriate procedure for testing the equality of a treatment means is the analysis of variance.

3-3.1 Decomposition of the Total Sum of Squares

The name **analysis of variance** is derived from a partitioning of total variability into its component parts. The total corrected sum of squares

$$SS_T = \sum_{i=1}^{a} \sum_{j=1}^{n} (y_{ij} - \bar{y}_{..})^2$$

is used as a measure of overall variability in the data. Intuitively, this is reasonable because, if we were to divide SS_T by the appropriate number of degrees of freedom (in this case, $an - 1 = N - 1$), we would have the **sample variance** of the y's. The sample variance is, of course, a standard measure of variability.

Note that the total corrected sum of squares SS_T may be written as

$$\sum_{i=1}^{a} \sum_{j=1}^{n} (y_{ij} - \bar{y}_{..})^2 = \sum_{i=1}^{a} \sum_{j=1}^{n} [(\bar{y}_{i.} - \bar{y}_{..}) + (y_{ij} - \bar{y}_{i.})]^2 \tag{3-4}$$

or

$$\sum_{i=1}^{a} \sum_{j=1}^{n} (y_{ij} - \bar{y}_{..})^2 = n \sum_{i=1}^{a} (\bar{y}_{i.} - \bar{y}_{..})^2 + \sum_{i=1}^{a} \sum_{j=1}^{n} (y_{ij} - \bar{y}_{i.})^2 + 2 \sum_{i=1}^{a} \sum_{j=1}^{n} (\bar{y}_{i.} - \bar{y}_{..})(y_{ij} - \bar{y}_{i.}) \tag{3-5}$$

However, the cross-product term in Equation 3-5 is zero, because

$$\sum_{j=1}^{n} (y_{ij} - \bar{y}_{i.}) = y_{i.} - n\bar{y}_{i.} = y_{i.} - n(y_{i.}/n) = 0$$

Therefore, we have

$$\sum_{i=1}^{a} \sum_{j=1}^{n} (y_{ij} - \bar{y}_{..})^2 = n \sum_{i=1}^{a} (\bar{y}_{i.} - \bar{y}_{..})^2 + \sum_{i=1}^{a} \sum_{j=1}^{n} (y_{ij} - \bar{y}_{i.})^2 \tag{3-6}$$

Equation 3-6 states that the total variability in the data, as measured by the total corrected sum of squares, can be partitioned into a sum of squares of the differences **between** the treatment averages and the grand average, plus a sum of squares of the differences of observations **within** treatments from the treatment average. Now, the difference between

[2] For more information on this subject, refer to the supplemental text material for Chapter 3.

the observed treatment averages and the grand average is a measure of the differences between treatment means, whereas the differences of observations within a treatment from the treatment average can be due only to random error. Thus, we may write Equation 3-6 symbolically as

$$SS_T = SS_{\text{Treatments}} + SS_E$$

where $SS_{\text{Treatments}}$ is called the sum of squares due to treatments (i.e., between treatments), and SS_E is called the sum of squares due to error (i.e., within treatments). There are $an = N$ total observations; thus, SS_T has $N - 1$ degrees of freedom. There are a levels of the factor (and a treatment means), so $SS_{\text{Treatments}}$ has $a - 1$ degrees of freedom. Finally, within any treatment there are n replicates providing $n - 1$ degrees of freedom with which to estimate the experimental error. Because there are a treatments, we have $a(n - 1) = an - a = N - a$ degrees of freedom for error.

It is helpful to examine explicitly the two terms on the right-hand side of the fundamental analysis of variance identity (Equation 3-6). Consider the error sum of squares

$$SS_E = \sum_{i=1}^{a}\sum_{j=1}^{n}(y_{ij} - \bar{y}_{i.})^2 = \sum_{i=1}^{a}\left[\sum_{j=1}^{n}(y_{ij} - \bar{y}_{i.})^2\right]$$

In this form it is easy to see that the term within square brackets, if divided by $n - 1$, is the sample variance in the ith treatment, or

$$S_i^2 = \frac{\sum_{j=1}^{n}(y_{ij} - \bar{y}_{i.})^2}{n - 1} \qquad i = 1, 2, \ldots, a$$

Now a sample variances may be combined to give a single estimate of the common population variance as follows:

$$\frac{(n-1)S_1^2 + (n-1)S_2^2 + \cdots + (n-1)S_a^2}{(n-1) + (n-1) + \cdots + (n-1)} = \frac{\sum_{i=1}^{a}\left[\sum_{j=1}^{n}(y_{ij} - \bar{y}_{i.})^2\right]}{\sum_{i=1}^{a}(n-1)} = \frac{SS_E}{(N-a)}$$

Thus, $SS_E/(N - a)$ is a pooled estimate of the common variance within each of the a treatments.

Similarly, if there were no differences between the a treatment means, we could use the variation of the treatment averages from the grand average to estimate σ^2. Specifically,

$$\frac{SS_{\text{Treatments}}}{a-1} = \frac{n\sum_{i=1}^{a}(\bar{y}_{i.} - \bar{y}_{..})^2}{a-1}$$

is an estimate of σ^2 if the treatment means are equal. The reason for this may be intuitively seen as follows: The quantity $\Sigma_{i=1}^{a}(\bar{y}_{i.} - \bar{y}_{..})^2/(a - 1)$ estimates σ^2/n, the variance

of the treatment averages, so $n\sum_{i=1}^{a}(\bar{y}_{i.} - \bar{y}_{..})^2/(a-1)$ must estimate σ^2 if there are no differences in treatment means.

We see that the analysis of variance identity (Equation 3-6) provides us with two estimates of σ^2—one based on the inherent variability within treatments and one based on the variability between treatments. If there are no differences in the treatment means, these two estimates should be very similar, and if they are not, we suspect that the observed difference must be caused by differences in the treatment means. Although we have used an intuitive argument to develop this result, a somewhat more formal approach can be taken.

The quantities

$$MS_{\text{Treatments}} = \frac{SS_{\text{Treatments}}}{a-1}$$

and

$$MS_E = \frac{SS_E}{N-a}$$

are called **mean squares**. We now examine the **expected values** of these mean squares. Consider

$$\begin{aligned} E(MS_E) = E\left(\frac{SS_E}{N-a}\right) &= \frac{1}{N-a}E\left[\sum_{i=1}^{a}\sum_{j=1}^{n}(y_{ij} - \bar{y}_{i.})^2\right] \\ &= \frac{1}{N-a}E\left[\sum_{i=1}^{a}\sum_{j=1}^{n}(y_{ij}^2 - 2y_{ij}\bar{y}_{i.} + \bar{y}_{i.}^2)\right] \\ &= \frac{1}{N-a}E\left[\sum_{i=1}^{a}\sum_{j=1}^{n}y_{ij}^2 - 2n\sum_{i=1}^{a}\bar{y}_{i.}^2 + n\sum_{i=1}^{a}\bar{y}_{i.}^2\right] \\ &= \frac{1}{N-a}E\left[\sum_{i=1}^{a}\sum_{j=1}^{n}y_{ij}^2 - \frac{1}{n}\sum_{i=1}^{a}y_{i.}^2\right] \end{aligned}$$

Substituting the model (Equation 3-1) into this equation, we obtain

$$E(MS_E) = \frac{1}{N-a}E\left[\sum_{i=1}^{a}\sum_{j=1}^{n}(\mu + \tau_i + \epsilon_{ij})^2 - \frac{1}{n}\sum_{i=1}^{a}\left(\sum_{j=1}^{n}\mu + \tau_i + \epsilon_{ij}\right)^2\right]$$

Now when squaring and taking expectation of the quantity within the brackets, we see that terms involving ϵ_{ij}^2 and $\epsilon_{i.}^2$ are replaced by σ^2 and $n\sigma^2$, respectively, because $E(\epsilon_{ij}) = 0$. Furthermore, all cross-products involving ϵ_{ij} have zero expectation. Therefore, after squaring and taking expectation, the last equation becomes

$$E(MS_E) = \frac{1}{N-a}\left[N\mu^2 + n\sum_{i=1}^{a}\tau_i^2 + N\sigma^2 - N\mu^2 - n\sum_{i=1}^{a}\tau_i^2 - a\sigma^2\right]$$

or

$$E(MS_E) = \sigma^2$$

By a similar approach, we may also show that[3]

$$E(MS_{\text{Treatments}}) = \sigma^2 + \frac{n\sum_{i=1}^{a}\tau_i^2}{a-1}$$

Thus, as we argued heuristically, $MS_E = SS_E/(N-a)$ estimates σ^2, and, if there are no differences in treatment means (which implies that $\tau_i = 0$), $MS_{\text{Treatments}} = SS_{\text{Treatments}}/(a-1)$ also estimates σ^2. However, note that if treatment means do differ, the expected value of the treatment mean square is greater than σ^2.

It seems clear that a test of the hypothesis of no difference in treatment means can be performed by comparing $MS_{\text{Treatments}}$ and MS_E. We now consider how this comparison may be made.

3-3.2 Statistical Analysis

We now investigate how a formal test of the hypothesis of no differences in treatment means ($H_0: \mu_1 = \mu_2 = \cdots = \mu_a$, or equivalently, $H_0: \tau_1 = \tau_2 = \cdots \tau_a = 0$) can be performed. Because we have assumed that the errors ϵ_{ij} are normally and independently distributed with mean zero and variance σ^2, the observations y_{ij} are normally and independently distributed with mean $\mu + \tau_i$ and variance σ^2. Thus, SS_T is a sum of squares in normally distributed random variables; consequently, it can be shown that SS_T/σ^2 is distributed as chi-square with $N-1$ degrees of freedom. Furthermore, we can show that SS_E/σ^2 is chi-square with $N-a$ degrees of freedom and that $SS_{\text{Treatments}}/\sigma^2$ is chi-square with $a-1$ degrees of freedom if the null hypothesis $H_0: \tau_i = 0$ is true. However, all three sums of squares are not necessarily independent because $SS_{\text{Treatments}}$ and SS_E add to SS_T. The following theorem, which is a special form of one attributed to William Cochran, is useful in establishing the independence of SS_E and $SS_{\text{Treatments}}$.

THEOREM 3-1

Cochran's Theorem

Let Z_i be NID(0, 1) for $i = 1, 2, \ldots, \nu$ and

$$\sum_{i=1}^{\nu} Z_i^2 = Q_1 + Q_2 + \cdots + Q_s$$

where $s \leq \nu$, and Q_i has ν_i degrees of freedom ($i = 1, 2, \ldots, s$). Then $Q_1, Q_2, \ldots, Q_s$ are independent chi-square random variables with $\nu_1, \nu_2, \ldots, \nu_s$ degrees of freedom, respectively, if and only if

$$\nu = \nu_1 + \nu_2 + \cdots + \nu_s$$

Because the degrees of freedom for $SS_{\text{Treatments}}$ and SS_E add to $N-1$, the total number of degrees of freedom, Cochran's theorem implies that $SS_{\text{Treatments}}/\sigma^2$ and SS_E/σ^2 are

[3] Refer to the supplemental text material for Chapter 3.

Table 3-3 The Analysis of Variance Table for the Single-Factor, Fixed Effects Model

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Between treatments	$SS_{\text{Treatments}} = n\sum_{i=1}^{a}(\bar{y}_{i.} - \bar{y}_{..})^2$	$a - 1$	$MS_{\text{Treatments}}$	$F_0 = \frac{MS_{\text{Treatments}}}{MS_E}$
Error (within treatments)	$SS_E = SS_T - SS_{\text{Treatments}}$	$N - a$	MS_E	
Total	$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{n}(y_{ij} - \bar{y}_{..})^2$	$N - 1$		

independently distributed chi-square random variables. Therefore, if the null hypothesis of no difference in treatment means is true, the ratio

$$F_0 = \frac{SS_{\text{Treatments}}/(a-1)}{SS_E/(N-a)} = \frac{MS_{\text{Treatments}}}{MS_E} \tag{3-7}$$

is distributed as F with $a - 1$ and $N - a$ degrees of freedom. Equation 3-7 is the **test statistic** for the hypothesis of no differences in treatment means.

From the expected mean squares we see that, in general, MS_E is an unbiased estimator of σ^2. Also, under the null hypothesis, $MS_{\text{Treatments}}$ is an unbiased estimator of σ^2. However, if the null hypothesis is false, the expected value of $MS_{\text{Treatments}}$ is greater than σ^2. Therefore, under the alternative hypothesis, the expected value of the numerator of the test statistic (Equation 3-7) is greater than the expected value of the denominator, and we should reject H_0 on values of the test statistic that are too large. This implies an upper-tail, one-tail critical region. Therefore, we should reject H_0 and conclude that there are differences in the treatment means if

$$F_0 > F_{\alpha,a-1,N-a}$$

where F_0 is computed from Equation 3-7. Alternatively, we could use the P-value approach for decision making.

Computing formulas for the sums of squares may be obtained by rewriting and simplifying the definitions of $MS_{\text{Treatments}}$ and SS_T in Equation 3-6. This yields

$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{n} y_{ij}^2 - \frac{y_{..}^2}{N} \tag{3-8}$$

and

$$SS_{\text{Treatments}} = \frac{1}{n}\sum_{i=1}^{a} y_{i.}^2 - \frac{y_{..}^2}{N} \tag{3-9}$$

The error sum of squares is obtained by subtraction as

$$SS_E = SS_T - SS_{\text{Treatments}} \tag{3-10}$$

The test procedure is summarized in Table 3-3 above. This is called an **analysis of variance table**.

EXAMPLE 3-1

The Tensile Strength Experiment

To illustrate the analysis of variance, return to the example first discussed in Section 3-1. Recall that the development engineer is interested in determining if the cotton weight

percentage in a synthetic fiber affects the tensile strength, and she has run a completely randomized experiment with five levels of cotton weight percentage and five replicates. For convenience, we repeat the data from Table 3-1 here:

Weight Percentage of Cotton	Observed Tensile Strength (lb/in^2)					Totals $y_{i.}$	Averages $\bar{y}_{i.}$
	1	2	3	4	5		
15	7	7	15	11	9	49	9.8
20	12	17	12	18	18	77	15.4
25	14	18	18	19	19	88	17.6
30	19	25	22	19	23	108	21.6
35	7	10	11	15	11	54	10.8
						$y_{..} = 376$	$\bar{y}_{..} = 15.04$

We will use the analysis of variance to test $H_0: \mu_1 = \mu_2 = \mu_3 = \mu_4 = \mu_5$ against the alternative H_1: some means are different. The sums of squares required are computed as follows:

$$SS_T = \sum_{i=1}^{5}\sum_{j=1}^{5} y_{ij}^2 - \frac{y_{..}^2}{N}$$

$$= (7)^2 + (7)^2 + (15)^2 + \cdots + (15)^2 + (11)^2 - \frac{(376)^2}{25} = 636.96$$

$$SS_{\text{Treatments}} = \frac{1}{n}\sum_{i=1}^{5} y_{i.}^2 - \frac{y_{..}^2}{N}$$

$$= \frac{1}{5}[(49)^2 + \cdots + (54)^2] - \frac{(376)^2}{25} = 475.76$$

$$SS_E = SS_T - SS_{\text{Treatments}}$$

$$= 636.96 - 475.76 = 161.20$$

Usually, these calculations would be performed on a computer, using a software package with the capability to analyze data from designed experiments.

The analysis of variance is summarized in Table 3-4. Note that the between-treatment mean square (118.94) is many times larger than the within-treatment or error mean square (8.06). This indicates that it is unlikely that the treatment means are equal. More formally, we can compute the F ratio $F_0 = 118.94/8.06 = 14.76$ and compare this to an appropriate upper-tail percentage point of the $F_{4,20}$ distribution. Suppose that the experimenter has selected $\alpha = 0.05$. From Appendix Table IV we find that $F_{0.05,4,20} = 2.87$. Because $F_0 = 14.76 > 2.87$, we reject H_0 and conclude that the treatment means differ; that is,

Table 3-4 Analysis of Variance for the Tensile Strength Data

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Cotton weight percentage	475.76	4	118.94	$F_0 = 14.76$	<0.01
Error	161.20	20	8.06		
Total	636.96	24			

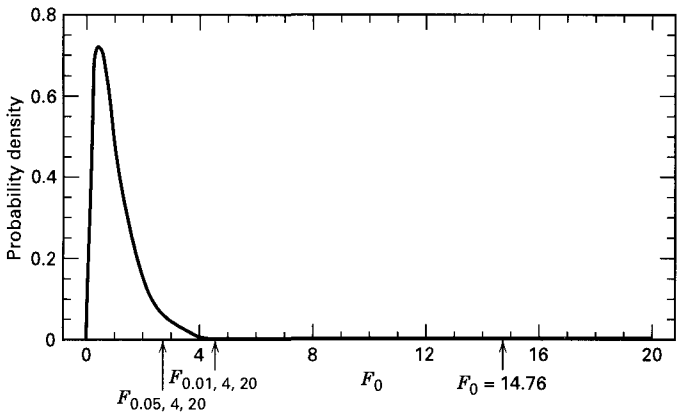


Figure 3-3 The reference distribution ($F_{4,20}$) for the test statistic F_0 in Example 3-1.

the cotton weight percentage in the fiber significantly affects the mean tensile strength. We could also compute a P-value for this test statistic. Figure 3-3 shows the reference distribution ($F_{4,20}$) for the test statistic F_0. Clearly, the P-value is very small in this case. Because $F_{0.01,4,20} = 4.43$ and $F_0 > 4.43$, we can conclude that an upper bound for the P-value is 0.01; that is, $P < 0.01$ (the exact P-value is $P = 9.11 \times 10^{-6}$).

Manual Computations

The reader has likely noted that we defined sum of squares in terms of averages; that is, from Equation 3-6,

$$SS_{\text{Treatments}} = n \sum_{i=1}^{a} (\bar{y}_{i.} - \bar{y}_{..})^2$$

but we developed the computing formulas using totals. For example, to compute $SS_{\text{Treatments}}$, we would use Equation 3-9:

$$SS_{\text{Treatments}} = \frac{1}{n} \sum_{i=1}^{a} y_{i.}^2 - \frac{y_{..}^2}{N}$$

The primary reason for this is convenience; furthermore, the totals $y_{i.}$ and $y_{..}$ are not as subject to rounding error as are the averages $\bar{y}_{i.}$ and $\bar{y}_{..}$.

Generally, we need not be too concerned with computing, because there are many widely available computer programs for performing the calculations. These computer programs are also helpful in performing many other analyses associated with experimental design (such as residual analysis and model adequacy checking). In many cases, these programs will also assist the experimenter in setting up the design.

When hand calculations are necessary, it is sometimes helpful to code the observations. This is illustrated in the next example.

EXAMPLE 3-2

Coding the Observations

The calculations in the analysis of variance may often be made more accurate or simplified by coding the observations. For example, consider the tensile strength data in

Table 3-5 Coded Tensile Strength Data for Example 3-2

Cotton Weight Percentage	Observations					Totals
	1	2	3	4	5	y_i
15	−8	−8	0	−4	−6	−26
20	−3	2	−3	3	3	2
25	−1	3	3	4	4	13
30	4	10	7	4	8	33
35	−8	−5	−4	0	−4	−21

Example 3-1. Suppose we subtract 15 from each observation. The coded data are shown in Table 3-5. It is easy to verify that

$$SS_T = (-8)^2 + (-8)^2 + \cdots + (-4)^2 - \frac{(1)^2}{25} = 636.96$$

$$SS_{\text{Treatments}} = \frac{(-26)^2 + (2)^2 + \cdots + (-21)^2}{5} - \frac{(1)^2}{25} = 475.76$$

and

$$SS_E = 161.20$$

Comparing these sums of squares to those obtained in Example 3-1, we see that subtracting a constant from the original data does not change the sums of squares.

Now suppose that we multiply each observation in Example 3-1 by 2. It is easy to verify that the sums of squares for the transformed data are $SS_T = 2547.84$, $SS_{\text{Treatments}} = 1903.04$, and $SS_E = 644.80$. These sums of squares appear to differ considerably from those obtained in Example 3-1. However, if they are divided by 4 (i.e., 2^2), the results are identical. For example, for the treatment sum of squares 1903.04/4 = 475.76. Also, for the coded data, the F ratio is $F = (1903.04/4)/(644.80/20) = 14.76$, which is identical to the F ratio for the original data. Thus, the analyses of variance are equivalent.

Randomization Tests and Analysis of Variance

In our development of the F test analysis of variance, we have used the assumption that the random errors ϵ_{ij} are normally and independently distributed random variables. The F test can also be justified as an approximation to a **randomization test**. To illustrate, suppose that we have five observations on each of two treatments and that we wish to test the equality of treatment means. The data would look like this:

Treatment 1	Treatment 2
y_{11}	y_{21}
y_{12}	y_{22}
y_{13}	y_{23}
y_{14}	y_{24}
y_{15}	y_{25}

We could use the F test analysis of variance to test $H_0: \mu_1 = \mu_2$. Alternatively, we could use a somewhat different approach. Suppose we consider all the possible ways of allo-

cating the 10 numbers in the sample above to the two treatments. There are 10!/5!5! = 252 possible arrangements of the 10 observations. If there is no difference in treatment means, all 252 arrangements are equally likely. For each of the 252 arrangements, we calculate the value of the F statistic using Equation 3-7. The distribution of these F values is called a **randomization distribution**, and a large value of F indicates that the data are not consistent with the hypothesis $H_0: \mu_1 = \mu_2$. For example, if the value of F actually observed was exceeded by only 5 of the values of the randomization distribution, this would correspond to rejection of $H_0: \mu_1 = \mu_2$ at a significance level of $\alpha = 5/252 = .0198$ (or 1.98 percent). Notice that no normality assumption is required in this approach.

The difficulty with this approach is that, even for relatively small problems, it is computationally prohibitive to enumerate the exact randomization distribution. However, numerous studies have shown that the exact randomization distribution is well-approximated by the usual normal-theory F distribution. Thus, even without the normality assumption, the F test can be viewed as an approximation to the randomization test. For further reading on randomization tests in the analysis of variance, see Box, Hunter, and Hunter (1978).

3-3.3 Estimation of the Model Parameters

We now present estimators for the parameters in the single-factor model

$$y_{ij} = \mu + \tau_i + \epsilon_{ij}$$

and confidence intervals on the treatment means. We will prove later that reasonable estimates of the overall mean and the treatment effects are given by

$$\begin{aligned} \hat{\mu} &= \bar{y}_{..} \\ \hat{\tau}_i &= \bar{y}_{i.} - \bar{y}_{..}, \qquad i = 1, 2, \ldots, a \end{aligned} \tag{3-11}$$

These estimators have considerable intuitive appeal; note that the overall mean is estimated by the grand average of the observations and that any treatment effect is just the difference between the treatment average and the grand average.

A **confidence interval** estimate of the ith treatment mean may be easily determined. The mean of the ith treatment is

$$\mu_i = \mu + \tau_i$$

A point estimator of μ_i would be $\hat{\mu}_i = \hat{\mu} + \hat{\tau}_i = \bar{y}_{i.}$. Now, if we assume that the errors are normally distributed, each $\bar{y}_{i.}$ is NID(μ_i, σ^2/n). Thus, if σ^2 were known, we could use the normal distribution to define the confidence interval. Using the MS_E as an estimator of σ^2, we would base the confidence interval on the t distribution. Therefore, a $100(1 - \alpha)$ percent confidence interval on the ith treatment mean μ_i is

$$\bar{y}_{i.} - t_{\alpha/2,N-a}\sqrt{\frac{MS_E}{n}} \leq \mu_i \leq \bar{y}_{i.} + t_{\alpha/2,N-a}\sqrt{\frac{MS_E}{n}} \tag{3-12}$$

A $100(1 - \alpha)$ percent confidence interval on the difference in any two treatments means, say $\mu_i - \mu_j$, would be

$$\bar{y}_{i.} - \bar{y}_{j.} - t_{\alpha/2,N-a}\sqrt{\frac{2MS_E}{n}} \leq \mu_i - \mu_j \leq \bar{y}_{i.} - \bar{y}_{j.} + t_{\alpha/2,N-a}\sqrt{\frac{2MS_E}{n}} \tag{3-13}$$

EXAMPLE 3-3

Using the data in Example 3-1, we may find the estimates of the overall mean and the treatment effects as $\hat{\mu} = 376/25 = 15.04$ and

$$\hat{\tau}_1 = \bar{y}_{1.} - \bar{y}_{..} = 9.80 - 15.04 = -5.24$$
$$\hat{\tau}_2 = \bar{y}_{2.} - \bar{y}_{..} = 15.40 - 15.04 = +0.36$$
$$\hat{\tau}_3 = \bar{y}_{3.} - \bar{y}_{..} = 17.60 - 15.04 = -2.56$$
$$\hat{\tau}_4 = \bar{y}_{4.} - \bar{y}_{..} = 21.60 - 15.04 = +6.56$$
$$\hat{\tau}_5 = \bar{y}_{5.} - \bar{y}_{..} = 10.80 - 15.04 = -4.24$$

A 95 percent confidence interval on the mean of treatment 4 (30 percent cotton) is computed from Equation 3-12 as

$$21.60 - 2.086\sqrt{\frac{8.06}{5}} \leq \mu_4 \leq 21.60 + 2.086\sqrt{\frac{8.06}{5}}$$

or

$$21.60 - 2.65 \leq \mu_4 \leq 21.60 + 2.65$$

Thus, the desired 95 percent confidence interval is $18.95 \leq \mu_4 \leq 24.25$.

Simultaneous Confidence Intervals

The confidence interval expressions given in Equations 3-12 and 3-13 are **one-at-a-time** confidence intervals. That is, the confidence level $1 - \alpha$ applies to only one particular estimate. However, in many problems, the experimenter may wish to calculate several confidence intervals, one for each of a number of means or differences between means. If there are r such $100(1 - \alpha)$ percent confidence intervals of interest, the probability that the r intervals will **simultaneously** be correct is at least $1 - r\alpha$. The probability $r\alpha$ is often called the **experimentwise error rate** or overall confidence coefficient. The number of intervals r does not have to be large before the set of confidence intervals becomes relatively uninformative. For example, if there are $r = 5$ intervals and $\alpha = 0.05$ (a typical choice), the simultaneous confidence level for the set of five confidence intervals is at least 0.75, and if $r = 10$ and $\alpha = 0.05$ the simultaneous confidence level is at least 0.50.

One approach to ensuring that the simultaneous confidence level is not too small is to replace $\alpha/2$ in the one-at-a-time confidence interval Equations 3-12 and 3-13 with $\alpha/(2r)$. This is called the **Bonferroni method**, and it allows the experimenter to construct a set of r simultaneous confidence intervals on treatment means or differences in treatment means for which the overall confidence level is at least $100(1 - \alpha)$ percent. When r is not too large, this is a very nice method that leads to reasonably short confidence intervals. For more information refer to the supplemental text material for Chapter 3.

3-3.4 Unbalanced Data

In some single-factor experiments the number of observations taken within each treatment may be different. We then say that the design is **unbalanced**. The analysis of variance described above may still be used, but slight modifications must be made in the

sum of squares formulas. Let n_i observations be taken under treatment i ($i = 1, 2, \ldots, a$) and $N = \sum_{i=1}^{a} n_i$. The manual computational formulas for SS_T and $SS_{\text{Treatments}}$ become

$$SS_T = \sum_{i=1}^{a} \sum_{j=1}^{n_i} y_{ij}^2 - \frac{y_{..}^2}{N} \tag{3-14}$$

and

$$SS_{\text{Treatments}} = \sum_{i=1}^{a} \frac{y_{i.}^2}{n_i} - \frac{y_{..}^2}{N} \tag{3-15}$$

No other changes are required in the analysis of variance.

There are two advantages in choosing a balanced design. First, the test statistic is relatively insensitive to small departures from the assumption of equal variances for the a treatments if the sample sizes are equal. This is not the case for unequal sample sizes. Second, the power of the test is maximized if the samples are of equal size.

3-4 MODEL ADEQUACY CHECKING

The decomposition of the variability in the observations through an analysis of variance identity (Equation 3-6) is a purely algebraic relationship. However, the use of the partitioning to test formally for no differences in treatment means requires that certain assumptions be satisfied. Specifically, these assumptions are that the observations are adequately described by the model

$$y_{ij} = \mu + \tau_i + \epsilon_{ij}$$

and that the errors are normally and independently distributed with mean zero and constant but unknown variance σ^2. If these assumptions are valid, the analysis of variance procedure is an exact test of the hypothesis of no difference in treatment means.

In practice, however, these assumptions will usually not hold exactly. Consequently, it is usually unwise to rely on the analysis of variance until the validity of these assumptions has been checked. Violations of the basic assumptions and model adequacy can be easily investigated by the examination of **residuals**. We define the residual for observation j in treatment i as

$$e_{ij} = y_{ij} - \hat{y}_{ij} \tag{3-16}$$

where $\hat{y}_{ij}$ is an estimate of the corresponding observation y_{ij} obtained as follows:

$$\begin{aligned} \hat{y}_{ij} &= \hat{\mu} + \hat{\tau}_i \\ &= \bar{y}_{..} + (\bar{y}_{i.} - \bar{y}_{..}) \\ &= \bar{y}_{i.} \end{aligned} \tag{3-17}$$

Equation 3-17 gives the intuitively appealing result that the estimate of any observation in the ith treatment is just the corresponding treatment average.

Examination of the residuals should be an automatic part of any analysis of variance. If the model is adequate, the residuals should be **structureless**; that is, they should contain no obvious patterns. Through a study of residuals, many types of model inadequacies and violations of the underlying assumptions can be discovered. In this section, we show how model diagnostic checking can be done easily by graphical analysis of residuals and how to deal with several commonly occurring abnormalities.

3-4.1 The Normality Assumption

A check of the normality assumption could be made by plotting a histogram of the residuals. If the NID(0, σ^2) assumption on the errors is satisfied, this plot should look like a sample from a normal distribution centered at zero. Unfortunately, with small samples, considerable fluctuation often occurs, so the appearance of a moderate departure from normality does not necessarily imply a serious violation of the assumptions. Gross deviations from normality are potentially serious and require further analysis.

An extremely useful procedure is to construct a normal probability plot of the residuals. Recall that in Chapter 2 we used a normal probability plot of the raw data to check the assumption of normality when using the *t*-test. In the analysis of variance, it is usually more effective (and straightforward) to do this with the residuals. If the underlying error distribution is normal, this plot will resemble a straight line. In visualizing the straight line, place more emphasis on the central values of the plot than on the extremes.

Table 3-6 shows the original data and the residuals for the tensile strength data in Example 3-1. The normal probability plot is shown in Figure 3-4 on the next page. The general impression from examining this display is that the error distribution may be slightly skewed, with the right tail being longer than the left. The tendency of the normal probability plot to bend down slightly on the left side implies that the left tail of the error distribution is somewhat *thinner* than would be anticipated in a normal distribution; that is, the negative residuals are not quite as large (in absolute value) as expected. This plot is not grossly nonnormal, however.

In general, moderate departures from normality are of little concern in the fixed effects analysis of variance (recall our discussion of randomization tests in Section 3-3.2). An error distribution that has considerably thicker or thinner tails than the normal is of more concern than a skewed distribution. Because the *F* test is only slightly affected, we say that the analysis of variance (and related procedures such as multiple comparisons) is **robust** to the normality assumption. Departures from normality usually cause both the true significance level and the power to differ slightly from the advertised values, with

Table 3-6 Data and Residuals from Example 3-1[a]

Weight Percentage of Cotton	Observations (j) 1	2	3	4	5	$\hat{y}_{ij} = \bar{y}_{i.}$
15	−2.8 7 (15)	−2.8 7 (19)	5.2 15 (25)	1.2 11 (12)	−0.8 9 (6)	9.8
20	−3.4 12 (8)	1.6 17 (14)	−3.4 12 (1)	2.6 18 (11)	2.6 19 (3)	15.4
25	−3.6 14 (18)	0.4 18 (13)	0.4 18 (20)	1.4 19 (7)	1.4 19 (9)	17.6
30	−2.6 19 (22)	3.4 25 (5)	0.4 22 (2)	−2.6 19 (24)	1.4 23 (10)	21.6
35	−3.8 7 (17)	−0.8 10 (21)	0.2 11 (4)	4.2 15 (16)	0.2 11 (23)	10.8

[a] The residuals are shown in the box in each cell. The numbers in parentheses indicate the order of data collection.

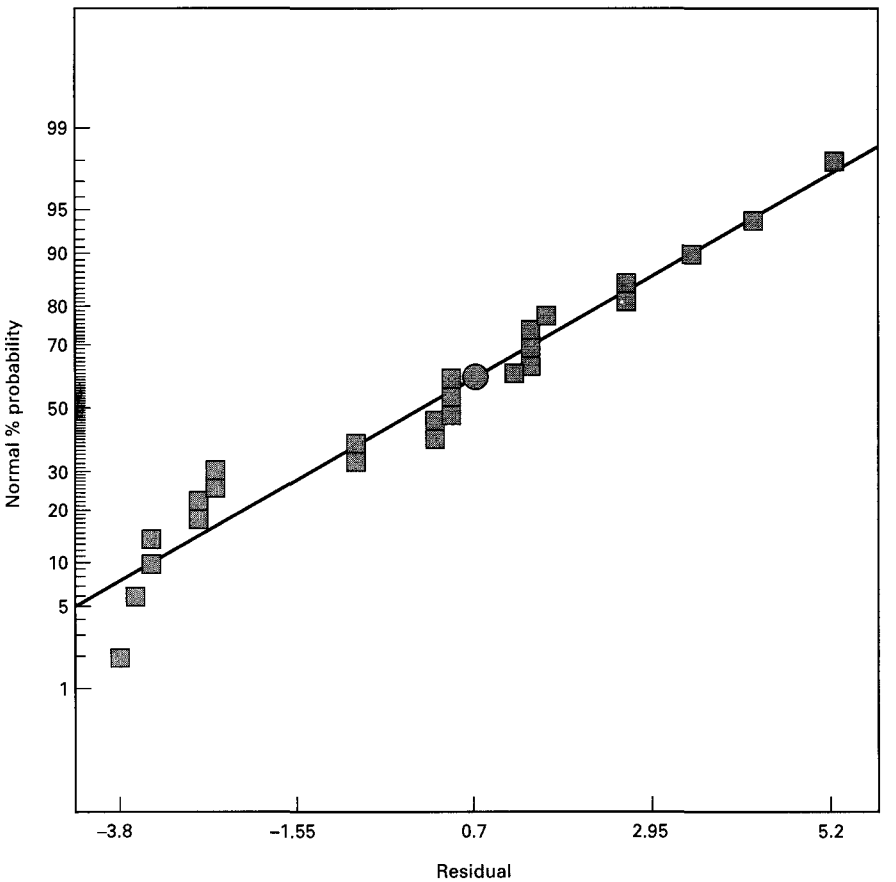


Figure 3-4 Normal probability plot of residuals for Example 3-1.

the power generally being lower. The random effects model that we will discuss in Chapter 12 is more severely affected by nonnormality.

A very common defect that often shows up on normal probability plots is one residual that is very much larger than any of the others. Such a residual is often called an **outlier**. The presence of one or more outliers can seriously distort the analysis of variance, so when a potential outlier is located, careful investigation is called for. Frequently, the cause of the outlier is a mistake in calculations or a data coding or copying error. If this is not the cause, the experimental circumstances surrounding this run must be carefully studied. If the outlying response is a particularly desirable value (high strength, low cost, etc.), the outlier may be more informative than the rest of the data. We should be careful not to reject or discard an outlying observation unless we have reasonably nonstatistical grounds for doing so. At worst, you may end up with two analyses; one with the outlier and one without.

There are several formal statistical procedures for detecting outliers [e.g., see Barnett and Lewis (1994), John and Prescott (1975), and Stefansky (1972)]. A rough check for outliers may be made by examining the **standardized residuals**

$$d_{ij} = \frac{e_{ij}}{\sqrt{MS_E}} \tag{3-18}$$

If the errors ϵ_{ij} are $N(0, \sigma^2)$, the standardized residuals should be approximately normal with mean zero and unit variance. Thus, about 68 percent of the standardized residuals should fall within the limits ± 1, about 95 percent of them should fall within ± 2, and virtually all of them should fall within ± 3. A residual bigger than 3 or 4 standard deviations from zero is a potential outlier.

For the tensile strength data of Example 3-1, the normal probability plot gives no indication of outliers. Furthermore, the largest standardized residual is

$$d_{13} = \frac{e_{13}}{\sqrt{MS_E}} = \frac{5.2}{\sqrt{8.06}} = \frac{5.2}{2.84} = 1.83$$

which should cause no concern.

3-4.2 Plot of Residuals in Time Sequence

Plotting the residuals in time order of data collection is helpful in detecting **correlation** between the residuals. A tendency to have runs of positive and negative residuals indicates positive correlation. This would imply that the **independence assumption** on the errors has been violated. This is a potentially serious problem and one that is difficult to correct, so it is important to prevent the problem if possible when the data are collected. Proper randomization of the experiment is an important step in obtaining independence.

Sometimes the skill of the experimenter (or the subjects) may change as the experiment progresses, or the process being studied may "drift" or become more erratic. This will often result in a change in the error variance over time. This condition often leads to a plot of residuals versus time that exhibits more spread at one end than at the other. Nonconstant variance is a potentially serious problem. We will have more to say on the subject in Sections 3-4.3 and 3-4.4.

Table 3-6 displays the residuals and the time sequence of data collection for the tensile strength data. A plot of these residuals versus time is shown in Figure 3-5. There

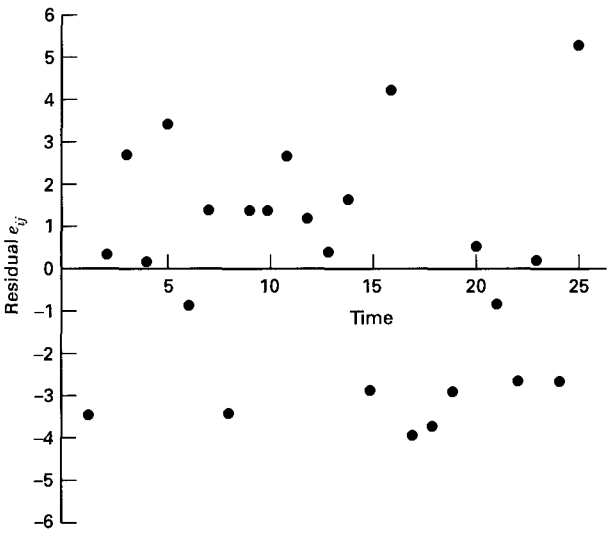


Figure 3-5 Plot of residuals versus time.

is no reason to suspect any violation of the independence or constant variance assumptions.

3-4.3 Plot of Residuals Versus Fitted Values

If the model is correct and if the assumptions are satisfied, the residuals should be structureless; in particular, they should be unrelated to any other variable including the predicted response. A simple check is to plot the residuals versus the fitted values $\hat{y}_{ij}$. (For the single-factor experiment model, remember that $\hat{y}_{ij} = \bar{y}_{i.}$, the ith treatment average.) This plot should not reveal any obvious pattern. Figure 3-6 plots the residuals versus the fitted values for the tensile strength data of Example 3-1. No unusual structure is apparent.

A defect that occasionally shows up on this plot is **nonconstant variance**. Sometimes the variance of the observations increases as the magnitude of the observation increases. This would be the case if the error or background noise in the experiment was a constant percentage of the size of the observation. (This commonly happens with many measuring instruments—error is a percentage of the scale reading.) If this were the case, the residuals would get larger as y_{ij} gets larger, and the plot of residuals versus $\hat{y}_{ij}$ would look like an outward-opening funnel or megaphone. Nonconstant variance also arises in cases where the data follow a nonnormal, skewed distribution because in skewed distributions the variance tends to be a function of the mean.

If the assumption of homogeneity of variances is violated, the F test is only slightly affected in the balanced (equal sample sizes in all treatments) fixed effects model. However, in unbalanced designs or in cases where one variance is very much larger than the others, the problem is more serious. Specifically, if the factor levels having the larger variances also have the smaller sample sizes, the actual type I error rate is larger than anticipated (or confidence intervals have lower actual confidence levels than were specified). Conversely, if the factor levels with larger variances also have the larger sample sizes, the significance levels are smaller than anticipated (confidence levels are higher). This is a good reason for choosing **equal sample sizes** whenever possible. For random

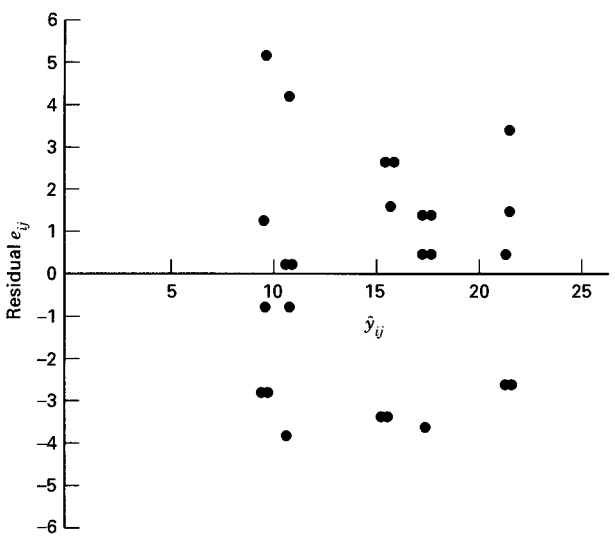


Figure 3-6 Plot of residuals versus fitted values.

effects models, unequal error variances can significantly disturb inferences on variance components even if balanced designs are used.

The usual approach to dealing with nonconstant variance when it occurs for the above reasons is to apply a **variance-stabilizing transformation** and then to run the analysis of variance on the transformed data. In this approach, one should note that the conclusions of the analysis of variance apply to the *transformed* populations.

Considerable research has been devoted to the selection of an appropriate transformation. If experimenters know the theoretical distribution of the observations, they may utilize this information in choosing a transformation. For example, if the observations follow the Poisson distribution, the **square root transformation** $y_{ij}^* = \sqrt{y_{ij}}$ or $y_{ij}^* = \sqrt{1 + y_{ij}}$ would be used. If the data follow the lognormal distribution, the **logarithmic transformation** $y_{ij}^* = \log y_{ij}$ is appropriate. For binomial data expressed as fractions, the **arcsin transformation** $y_{ij}^* = \arcsin\sqrt{y_{ij}}$ is useful. When there is no obvious transformation, the experimenter usually *empirically* seeks a transformation that equalizes the variance regardless of the value of the mean. We offer some guidance on this at the conclusion of this section. In factorial experiments, which we introduce in Chapter 5, another approach is to select a transformation that minimizes the interaction mean square, resulting in an experiment that is easier to interpret. In Chapter 14, we discuss in more detail methods for analytically selecting the form of the transformation. Transformations made for inequality of variance also affect the form of the error distribution. In most cases, the transformation brings the error distribution closer to normal. For more discussion of transformations, refer to Bartlett (1947), Box and Cox (1964), Dolby (1963), and Draper and Hunter (1969).

Statistical Tests for Equality of Variance

Although residual plots are frequently used to diagnose inequality of variance, several statistical tests have also also been proposed. These tests may be viewed as formal tests of the hypotheses

$$H_0: \sigma_1^2 = \sigma_2^2 = \cdots = \sigma_a^2$$
$$H_1: \text{above not true for at least one } \sigma_i^2$$

A widely used procedure is **Bartlett's test**. The procedure involves computing a statistic whose sampling distribution is closely approximated by the chi-square distribution with $a - 1$ degrees of freedom when the a random samples are from independent normal populations. The test statistic is

$$\chi_0^2 = 2.3026 \frac{q}{c} \tag{3-19}$$

where

$$q = (N - a)\log_{10} S_p^2 - \sum_{i=1}^{a} (n_i - 1)\log_{10} S_i^2$$

$$c = 1 + \frac{1}{3(a-1)}\left(\sum_{i=1}^{a} (n_i - 1)^{-1} - (N - a)^{-1}\right)$$

$$S_p^2 = \frac{\sum_{i=1}^{a} (n_i - 1)S_i^2}{N - a}$$

and S_i^2 is the sample variance of the ith population.

The quantity q is large when the sample variances S_i^2 differ greatly and is equal to zero when all S_i^2 are equal. Therefore, we should reject H_0 on values of χ_0^2 that are too large; that is, we reject H_0 only when

$$\chi_0^2 > \chi_{\alpha,a-1}^2$$

where $\chi_{\alpha,a-1}^2$ is the upper α percentage point of the chi-square distribution with $a - 1$ degrees of freedom. The P-value approach to decision making could also be used.

Bartlett's test is very sensitive to the normality assumption. Consequently, when the validity of this assumption is doubtful, Bartlett's test should not be used.

EXAMPLE 3-4

Because the normality assumption is not in question, we can apply Bartlett's test to the tensile strength data from the cotton weight percentage experiment in Example 3-1. We first compute the sample variances in each treatment and find that $S_1^2 = 11.2$, $S_2^2 = 9.8$, $S_3^2 = 4.3$, $S_4^2 = 6.8$, and $S_5^2 = 8.2$. Then

$$S_p^2 = \frac{4(11.2) + 4(9.8) + 4(4.3) + 4(6.8) + 4(8.2)}{20} = 8.06$$

$$q = 20 \log_{10}(8.06) - 4[\log_{10}11.2 + \log_{10}9.8 + \log_{10} 4.3 + \log_{10}6.8 + \log_{10}8.2]$$
$$= 0.45$$

$$c = 1 + \frac{1}{3(4)}\left(\frac{5}{4} - \frac{1}{20}\right) = 1.10$$

and the test statistic is

$$\chi_0^2 = 2.3026 \frac{(0.45)}{(1.10)} = 0.93$$

Because $\chi_{0.05,4}^2 = 9.49$, we cannot reject the null hypothesis and conclude that all five variances are the same. This is the same conclusion reached by analyzing the plot of residuals versus fitted values.

Because Bartlett's test is sensitive to the normality assumption, there may be situations where an alternative procedure would be useful. Anderson and McLean (1974) present a nice discussion of statistical tests for equality of variance. The **modified Levene test** [see Levene (1960) and Conover, Johnson, and Johnson (1981)] is a very nice procedure that is robust to departures from normality. To test the hypothesis of equal variances in all treatments, the modified Levene test uses the absolute deviation of the observations y_{ij} in each treatment from the treatment median, say $\tilde{y}_i$. Denote these deviations by

$$d_{ij} = |y_{ij} - \tilde{y}_i| \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, n_i \end{cases}$$

The modified Levene test then evaluates whether or not the mean of these deviations are equal for all treatments. It turns out that if the mean deviations are equal, the variances of the observations in all treatments will be the same. The test statistic for Levene's test

Table 3-7 Peak Discharge Data

Estimation Method	Observations						$\bar{y}_{i.}$	$\tilde{y}_i$	S_i
1	0.34	0.12	1.23	0.70	1.75	0.12	0.71	0.520	0.66
2	0.91	2.94	2.14	2.36	2.86	4.55	2.63	2.610	1.09
3	6.31	8.37	9.75	6.09	9.82	7.24	7.93	7.805	1.66
4	17.15	11.82	10.95	17.20	14.35	16.82	14.72	15.59	2.77
Estimation Method	Deviations d_{ij} for the Modified Levene Test								
1	0.18	0.40	0.71	0.18	1.23	0.40			
2	1.70	0.33	0.47	0.25	0.25	1.94			
3	1.495	0.565	1.945	1.715	2.015	0.565			
4	1.56	3.77	4.64	1.61	1.24	1.23			

is simply the usual ANOVA F statistic for testing equality of means applied to the absolute deviations.

EXAMPLE 3-5

A civil engineer is interested in determining whether four different methods of estimating flood flow frequency produce equivalent estimates of peak discharge when applied to the same watershed. Each procedure is used six times on the watershed, and the resulting discharge data (in cubic feet per second) are shown in the upper panel of Table 3-7. The analysis of variance for the data, summarized in Table 3-8, implies that there is a difference in mean peak discharge estimates given by the four procedures. The plot of residuals versus fitted values, shown in Figure 3-7 (top of page 84), is disturbing because the outward-opening funnel shape indicates that the constant variance assumption is not satisfied.

We will apply the modified Levene test to the peak discharge data. The upper panel of Table 3-7 contains the treatment medians $\tilde{y}_i$ and the lower panel contains the deviations d_{ij} around the medians. Levene's test consists of conducting a standard analysis of variance on the d_{ij}. The F test statistic that results from this is $F_0 = 4.55$, for which the P-value is $P = 0.0137$. Therefore, Levene's test rejects the null hypothesis of equal variances, essentially confirming the diagnosis we made from visual examination of Figure 3-7. The peak discharge data is a good candidate for data transformation.

Empirical Selection of a Transformation

We observed above that, if experimenters knew the relationship between the variance of the observations and the mean, they could use this information to guide them in selecting

Table 3-8 Analysis of Variance for Peak Discharge Data

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Methods	708.3471	3	236.1157	76.07	<0.001
Error	62.0811	20	3.1041		
Total	770.4282	23			

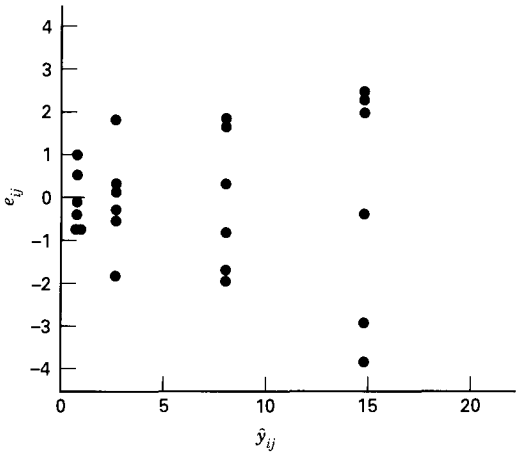


Figure 3-7 Plot of residuals versus $\hat{y}_{ij}$ for Example 3-5.

the form of the transformation. We now elaborate on this point and show one method for empirically selecting the form of the required transformation from the data.

Let $E(y) = \mu$ be the mean of y, and suppose that the standard deviation of y is proportional to a power of the mean of y such that

$$\sigma_y \propto \mu^{\alpha}$$

We want to find a transformation on y that yields a constant variance. Suppose that the transformation is a power of the original data, say

$$y^* = y^{\lambda} \tag{3-20}$$

Then it can be shown that

$$\sigma_{y^*} \propto \mu^{\lambda+\alpha-1} \tag{3-21}$$

Clearly, if we set $\lambda = 1 - \alpha$, the variance of the transformed data y^* is constant.

Several of the common transformations discussed previously are summarized in Table 3-9. Note that $\lambda = 0$ implies the log transformation. These transformations are arranged in order of increasing **strength**. By the strength of a transformation we mean the amount of curvature it induces. A mild transformation applied to data spanning a narrow

Table 3-9 Variance-Stabilizing Transformations

Relationship Between σ_y and μ	α	$\lambda = 1 - \alpha$	Transformation	Comment
$\sigma_y \propto$ constant	0	1	No transformation	
$\sigma_y \propto \mu^{1/2}$	1/2	1/2	Square root	Poisson (count) data
$\sigma_y \propto \mu$	1	0	Log	
$\sigma_y \propto \mu^{3/2}$	3/2	−1/2	Reciprocal square root	
$\sigma_y \propto \mu^2$	2	−1	Reciprocal	

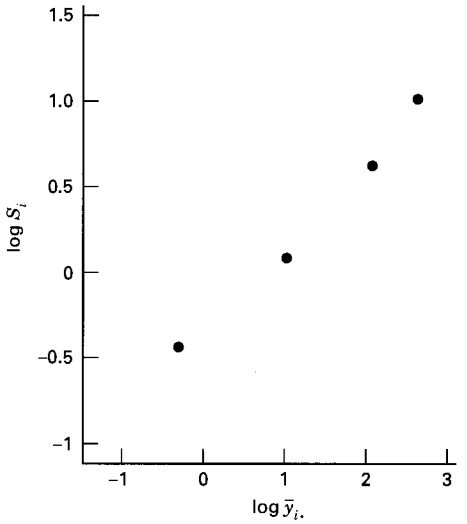


Figure 3-8 Plot of log S_i versus log $\bar{y}_{i.}$ for the peak discharge data from Example 3-5.

range has little effect on the analysis, whereas a strong transformation applied over a large range may have dramatic results. Transformations often have little effect unless the ratio y_{max}/y_{min} is larger than 2 or 3.

In many experimental design situations where there is replication, we can empirically estimate α from the data. Because in the ith treatment combination $\sigma_{y_i} \propto \mu_i^{\alpha} = \theta\mu_i^{\alpha}$, where θ is a constant of proportionality, we may take logs to obtain

$$\log \sigma_{y_i} = \log \theta + \alpha \log \mu_i \tag{3-22}$$

Therefore, a plot of log σ_{y_i} versus log μ_i would be a straight line with slope α. Because we don't know σ_{y_i} and μ_i, we may substitute reasonable estimates of them in Equation 3-22 and use the slope of the resulting straight line fit as an estimate of α. Typically, we would use the standard deviation S_i and the average $\bar{y}_{i.}$ of the ith treatment (or, more generally, the ith treatment combination or set of experimental conditions) to estimate σ_{y_i} and μ_i.

To investigate the possibility of using a variance-stabilizing transformation on the peak discharge data from Example 3-5, we plot log S_i versus log $\bar{y}_{i.}$ in Figure 3-8. The slope of a straight line passing through these four points is close to 1/2 and, from Table 3-9, this implies that the square root transformation may be appropriate. The analysis of variance for the transformed data $y^* = \sqrt{y}$ is presented in Table 3-10, and a plot of

Table 3-10 Analysis of Variance for Transformed Peak Discharge Data, $y^* = \sqrt{y}$

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Methods	32.6842	3	10.8947	76.99	<0.001
Error	2.6884	19	0.1415		
Total	35.3726	22			

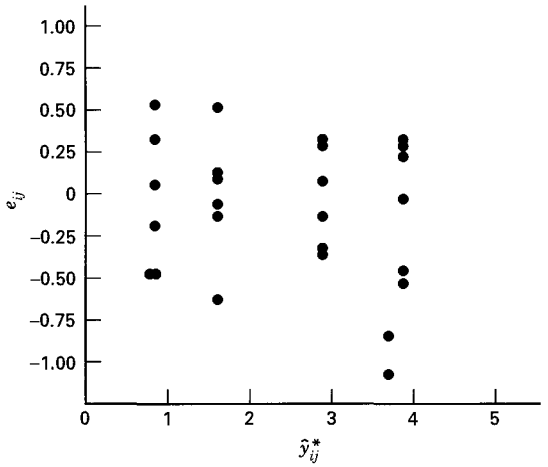


Figure 3-9 Plot of residuals from transformed data versus $\hat{y}_{ij}^*$ for the peak discharge data in Example 3-5.

residuals versus the predicted response is shown in Figure 3-9. This residual plot is much improved in comparison to Figure 3-7, so we conclude that the square root transformation has been helpful. Note that in Table 3-10 we have reduced the error degrees of freedom by 1 to account for the use of the data to estimate the transformation parameter α.

In practice, many experimenters select the form of the transformation by simply trying several alternatives and observing the effect of each transformation on the plot of residuals versus the predicted response. The transformation that produced the most satisfactory residual plot is then selected.

3-4.4 Plots of Residuals Versus Other Variables

If data have been collected on any other variables that might possibly affect the response, the residuals should be plotted against these variables. For example, in the tensile strength experiment of Example 3-1, strength may be significantly affected by the thickness of the fiber, so the residuals should be plotted versus fiber thickness. If different testing machines were used to collect the data, the residuals should be plotted against machines. Patterns in such residual plots imply that the variable affects the response. This suggests that the variable should be either controlled more carefully in future experiments or included in the analysis.

3-5 PRACTICAL INTERPRETATION OF RESULTS

After conducting the experiment, performing the statistical analysis, and investigating the underlying assumptions, the experimenter is ready to draw practical conclusions about the problem he or she is studying. Often this is relatively easy, and certainly in the simple experiments we have considered so far, this might be done somewhat informally, perhaps by inspection of graphical displays such as the box plots and scatter diagram in Figures 3-1 and 3-2. However, in some cases, more formal techniques need to be applied. We will present some of these techniques in this section.

3-5.1 A Regression Model

The factors involved in an experiment can be either **quantitative** or **qualitative**. A quantitative factor is one whose levels can be associated with points on a numerical scale, such as temperature, pressure, or time. Qualitative factors, on the other hand, are factors for which the levels cannot be arranged in order of magnitude. Operators, batches of raw material, and shifts are typical qualitative factors because there is no reason to rank them in any particular numerical order.

Insofar as the initial design and analysis of the experiment are concerned, both types of factors are treated identically. The experimenter is interested in determining the differences, if any, between the levels of the factors. If the factor is qualitative, such as operators, it is meaningless to consider the response for a subsequent run at an intermediate level of the factor. However, with a quantitative factor such as time, the experimenter is usually interested in the entire range of values used, particularly the response from a subsequent run at an intermediate factor level. That is, if the levels 1.0, 2.0, and 3.0 hours are used in the experiment, we may wish to predict the response at 2.5 hours. Thus, the experimenter is frequently interested in developing an interpolation equation for the response variable in the experiment. This equation is an **empirical model** of the process that has been studied.

The general approach to fitting empirical models is called **regression analysis**, which is discussed extensively in Chapter 10. See also the supplemental text material for this chapter. This section briefly illustrates the technique using the tensile strength data of Example 3-1.

Figure 3-10 presents a scatter diagram of tensile strength y versus the weight percentage of cotton x in the fabric for the experiment in Example 3-1. The open circles on the graph are the mean tensile strengths at each value of cotton weight percentage x. From examining the scatter diagram, it is clear that the relationship between tensile

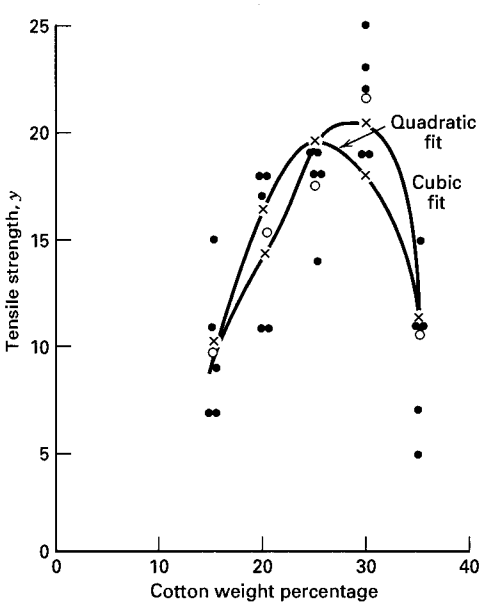


Figure 3-10 Scatter diagram for the tensile strength data of Example 3-1.

strength and weight percentage cotton is not linear. As a first approximation, we could try fitting a **quadratic model** to the data, say

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$$

where β_0, β_1, and β_2 are unknown parameters to be estimated and ϵ is a random error term. The method often used to estimate the parameters in a model such as this is the method of least squares. This consists of choosing estimates of the β's such that the sum of the squares of the errors (the ϵ's) are minimized. The least squares fit in our example is

$$\hat{y} = -39.9886 + 4.596x - 0.0886x^2$$

(If you are unfamiliar with regression methods, see Chapter 10 and the supplemental text material for this chapter.)

This quadratic model is shown in Figure 3-10. It does not appear to be very satisfactory because it drastically underestimates the responses at $x = 30$ percent cotton and overestimates the responses at $x = 25$ percent. Perhaps an improvement can be obtained by adding a cubic term in x. The resulting **cubic model** fit is

$$\hat{y} = 62.6114 - 9.0114x + 0.4814x^2 - 0.0076x^3$$

This cubic fit is also shown in Figure 3-10. The cubic model appears to be superior to the quadratic because it provides a better fit at $x = 25$ and $x = 30$ percent cotton.

In general, we would like to fit the lowest-order polynomial that adequately describes the system or process. In this example, the cubic polynomial seems to fit better than the quadratic, so the extra complexity of the cubic model is justified. Selecting the order of the approximating polynomial is not always easy, however, and it is relatively easy to overfit, that is, to add high-order polynomial terms that do not really improve the fit but increase the complexity of the model and often damage its usefulness as a predictor or interpolation equation.

In this example, the empirical model could be used to predict mean tensile strength at values of cotton weight percentage within the region of experimentation. In other cases, the empirical model could be used for **process optimization**, that is, finding the levels of the design variables that result in the best values of the response. We will discuss and illustrate these problems extensively later in the book.

3-5.2 Comparisons Among Treatment Means

Suppose that in conducting an analysis of variance for the fixed effects model the null hypothesis is rejected. Thus, there are differences between the treatment means, but exactly *which* means differ is not specified. Sometimes in this situation, further comparisons and analysis among **groups** of treatment means may be useful. The ith treatment mean is defined as $\mu_i = \mu + \tau_i$, and μ_i is estimated by $\bar{y}_{i.}$. Comparisons between treatment means are made in terms of either the treatment totals $\{y_{i.}\}$ or the treatment averages $\{\bar{y}_{i.}\}$. The procedures for making these comparisons are usually called **multiple comparison methods**. In the next several sections, we discuss methods for making comparisons among individual treatment means or groups of these means.

3-5.3 Graphical Comparisons of Means

It is very easy to develop a graphical procedure for the comparison of means following an analysis of variance. Suppose that the factor of interest has a levels and that $\bar{y}_{1.}, \bar{y}_{2.}, \ldots, \bar{y}_{a.}$ are the treatment averages. If we know σ, any treatment average would have a standard deviation $\sigma/\sqrt{n}$. Consequently, if all factor level means are identical, the observed sample means $\bar{y}_{i.}$ would behave as if they were a set of observations drawn at random from a normal distribution with mean $\bar{y}_{..}$ and standard deviation $\sigma/\sqrt{n}$. Visualize a normal distribution capable of being slid along an axis below which the $\bar{y}_{1.}, \bar{y}_{2.}, \ldots, \bar{y}_{a.}$ are plotted. If the treatment means are all equal, there should be some position for this distribution that makes it obvious that the $\bar{y}_{i.}$ values were drawn from the same distribution. If this is not the case, the $\bar{y}_{i.}$ values that appear *not* to have been drawn from this distribution are associated with factor levels that produce different mean responses.

The only flaw in this logic is that σ is unknown. However, we can replace σ with $\sqrt{MS_E}$ from the analysis of variance and use a t distribution with a scale factor $\sqrt{MS_E/n}$ instead of the normal. Such an arrangement for the tensile strength data of Example 3-1 is shown in Figure 3-11.

To sketch the t distribution in Figure 3-11, simply multiply the abscissa t value by the scale factor

$$\sqrt{MS_E/n} = \sqrt{8.06/5} = 1.27$$

and plot this against the ordinate of t at that point. Because the t distribution looks much like the normal, except that it is a little flatter near the center and has longer tails, this sketch is usually easily constructed by eye. If you wish to be more precise, there is a table of abscissa t values and the corresponding ordinates in Box, Hunter, and Hunter (1978). The distribution can have an arbitrary origin, although it is usually best to choose one in the region of the $\bar{y}_{i.}$ values to be compared. In Figure 3-11, the origin is 15 lb/in^2.

Now visualize sliding the t distribution in Figure 3-11 along the horizontal axis, and examine the five means plotted in the figure. Notice that there is no location for the distribution such that all five averages could be thought of as typical, randomly selected observations from the distribution. This implies that all five means are not equal; thus, the figure is a graphical display of the results of the analysis of variance. The figure does indicate that 30 percent cotton produces much higher tensile strengths than would 20 or 25 percent cotton (which are about the same) or that either 15 or 35 percent cotton (which are about the same) would result in even lower tensile strengths.

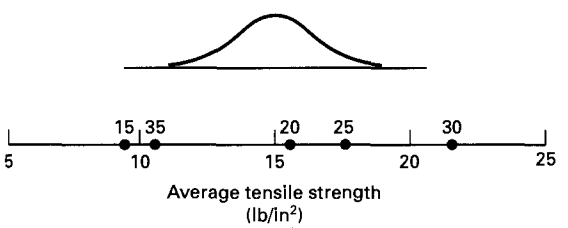


Figure 3-11 Tensile strength averages from the cotton weight percentage experiment in relation to a t distribution with a scale factor $\sqrt{MS_E/n} = \sqrt{8.06/5} = 1.27$.

This simple procedure is a rough but effective technique for many multiple comparison problems. However, there are more formal methods. We now give a brief discussion of some of these procedures.

3-5.4 Contrasts

Many multiple comparison methods use the idea of a contrast. Consider the synthetic fiber testing problem of Example 3-1. Because the null hypothesis was rejected, we know that some cotton weight percentages produce different tensile strengths than others, but which ones actually cause this difference? We might suspect at the outset of the experiment that levels 4 and 5 cotton weight percentages (30 and 35 percent) produce the same tensile strength, implying that we would like to test the hypothesis

$$H_0: \mu_4 = \mu_5$$
$$H_1: \mu_4 \neq \mu_5$$

or equivalently,

$$H_0: \mu_4 - \mu_5 = 0$$
$$H_1: \mu_4 - \mu_5 \neq 0 \tag{3-23}$$

If we had suspected at the start of the experiment that the *average* of the lowest levels of cotton weight percentages (1 and 2) did not differ from the *average* of the highest levels of cotton weight percentages (4 and 5), then the hypothesis would have been

$$H_0: \mu_1 + \mu_2 = \mu_4 + \mu_5$$
$$H_1: \mu_1 + \mu_2 \neq \mu_4 + \mu_5$$

or

$$H_0: \mu_1 + \mu_2 - \mu_4 - \mu_5 = 0$$
$$H_1: \mu_1 + \mu_2 - \mu_4 - \mu_5 = 0 \tag{3-24}$$

In general, a **contrast** is a linear combination of parameters of the form

$$\Gamma = \sum_{i=1}^{a} c_i \mu_i$$

where the **contrast constant** $c_1, c_2, \ldots, c_a$ sum to zero; that is, $\Sigma_{i=1}^{a} c_i = 0$. Both of the hypotheses above can be expressed in terms of contrasts:

$$H_0: \sum_{i=1}^{a} c_i \mu_i = 0$$
$$H_1: \sum_{i=1}^{a} c_i \mu_i \neq 0 \tag{3-25}$$

The contrast constants for the hypotheses in Equation 3-23 are $c_1 = c_2 = c_3 = 0, c_4 = +1$, and $c_5 = -1$, whereas for the hypotheses in Equation 3-24 they are $c_1 = c_2 = +1$, $c_3 = 0$, and $c_4 = c_5 = -1$.

Testing hypotheses involving contrasts can be done in two basic ways. The first method uses a t-test. Write the contrast of interest in terms of the **treatment totals**, giving

$$C = \sum_{i=1}^{a} c_i y_{i.}$$

The variance of C is

$$V(C) = n\sigma^2 \sum_{i=1}^{a} c_i^2 \tag{3-26}$$

when the sample sizes in each treatment are equal. If the null hypothesis in Equation 3-25 is true, the ratio

$$\frac{\sum_{i=1}^{a} c_i y_{i.}}{\sqrt{n\sigma^2 \sum_{i=1}^{a} c_i^2}}$$

has the $N(0, 1)$ distribution. Now we would replace the unknown variance σ^2 by its estimate, the mean square error MS_E and use the statistic

$$t_0 = \frac{\sum_{i=1}^{a} c_i y_{i.}}{\sqrt{nMS_E \sum_{i=1}^{a} c_i^2}} \tag{3-27}$$

to test the hypotheses in Equation 3-25. The null hypothesis would be rejected if $|t_0|$ in Equation 3-27 exceeds $t_{\alpha/2,N-a}$.

The second approach uses an F test. Now the square of a t random variable with ν degrees of freedom is an F random variable with 1 numerator and ν denominator degrees of freedom. Therefore, we can obtain

$$F_0 = t_0^2 = \frac{\left(\sum_{i=1}^{a} c_i y_{i.}\right)^2}{nMS_E \sum_{i=1}^{a} c_i^2} \tag{3-28}$$

as an F statistic for testing Equation 3-25. The null hypothesis would be rejected if $F_0 > F_{\alpha,1,N-a}$. We can write the test statistic of Equation 3-28 as

$$F_0 = \frac{MS_C}{MS_E} = \frac{SS_C/1}{MS_E}$$

where the single degree of freedom contrast sum of squares is

$$SS_C = \frac{\left(\sum_{i=1}^{a} c_i y_{i.}\right)^2}{n \sum_{i=1}^{a} c_i^2} \tag{3-29}$$

Confidence Interval for a Contrast

Instead of testing hypotheses about a contrast, it may be more useful to construct a confidence interval. The contrast is then often written in terms of treatment averages $\bar{y}_{i.}$. Suppose that the contrast of interest is

$$\Gamma = \sum_{i=1}^{a} c_i \mu_i$$

Replacing the treatment means with the treatment averages yields

$$C = \sum_{i=1}^{a} c_i \bar{y}_{i.}$$

and

$$V(C) = \frac{\sigma^2}{n} \sum_{i=1}^{a} c_i^2$$

when the sample sizes are equal. If we use MS_E to estimate σ^2, the $100(1 - \alpha)$ percent confidence interval on the contrast $\Sigma_{i=1}^{a} c_i \mu_i$ is

$$\sum_{i=1}^{a} c_i \bar{y}_{i.} - t_{\alpha/2,N-a} \sqrt{\frac{MS_E}{n} \sum_{i=1}^{a} c_i^2} \leq \sum_{i=1}^{a} c_i \mu_i \leq \sum_{i=1}^{a} c_i \bar{y}_{i.} + t_{\alpha/2,N-a} \sqrt{\frac{MS_E}{n} \sum_{i=1}^{a} c_i^2} \quad (3\text{-}30)$$

Clearly if this confidence interval includes zero, we would be unable to reject the null hypothesis in Equation 3-25.

Standardized Contrast

When more than one contrast is of interest, it is often useful to evaluate them on the same scale. One way to do this is to standardize the contrast so that it has variance σ^2. If the contrast $\Sigma_{i=1}^{a} c_i \mu_i$ is written in terms of treatment totals as $\Sigma_{i=1}^{a} c_i y_{i.}$, dividing it by $\sqrt{n \Sigma_{i=1}^{a} c_i^2}$ will produce a standardized contrast with variance σ^2. Effectively, then, the **standardized contrast** is

$$\sum_{i=1}^{a} c_i^* y_{i.}$$

where

$$c_i^* = \frac{c_i}{\sqrt{n \sum_{i=1}^{a} c_i^2}}$$

Unequal Sample Sizes

When the sample sizes in each treatment are different, minor modifications are made in the above results. First, note that the definition of a contrast now requires that

$$\sum_{i=1}^{a} n_i c_i = 0$$

Other required changes are straightforward. For example, the t statistic in Equation 3-27 becomes

$$t_0 = \frac{\sum_{i=1}^{a} c_i y_{i.}}{\sqrt{MS_E \sum_{i=1}^{a} n_i c_i^2}}$$

and the contrast sum of squares from Equation 3-29 becomes

$$SS_C = \frac{\left(\sum_{i=1}^{a} c_i y_{i.}\right)^2}{\sum_{i=1}^{a} n_i c_i^2}$$

3-5.5 Orthogonal Contrasts

A useful special case of the procedure in Section 3-5.4 is that of **orthogonal contrasts**. Two contrasts with coefficients $\{c_i\}$ and $\{d_i\}$ are orthogonal if

$$\sum_{i=1}^{a} c_i d_i = 0$$

or, for an unbalanced design, if

$$\sum_{i=1}^{a} n_i c_i d_i = 0$$

For a treatments the set of $a - 1$ orthogonal contrasts partition the sum of squares due to treatments into $a - 1$ independent single-degree-of-freedom components. Thus, tests performed on orthogonal contrasts are independent.

There are many ways to choose the orthogonal contrast coefficients for a set of treatments. Usually, something in the nature of the experiment should suggest which comparisons will be of interest. For example, if there are $a = 3$ treatments, with treatment 1 a control and treatments 2 and 3 actual levels of the factor of interest to the experimenter, appropriate orthogonal contrasts might be as follows:

Treatment	Coefficients for Orthogonal Contrasts	
1 (control)	−2	0
2 (level 1)	1	−1
3 (level 2)	1	1

Note that contrast 1 with $c_i = -2, 1, 1$ compares the average effect of the factor with the control, whereas contrast 2 with $d_i = 0, -1, 1$ compares the two levels of the factor of interest.

Generally, the method of contrasts (or orthogonal contrasts) is useful for what are called **preplanned comparisons**. That is, the contrasts are specified prior to running the

experiment and examining the data. The reason for this is that, if comparisons are selected after examining the data, most experimenters would construct tests that correspond to large observed differences in means. These large differences could be the result of the presence of real effects or they could be the result of random error. If experimenters consistently pick the largest differences to compare, they will inflate the type I error of the test because it is likely that, in an unusually high percentage of the comparisons selected, the observed differences will be the result of error. Examining the data to select comparisons of potential interest is often called **data snooping**. The Scheffé method for all comparisons, discussed in the next section, permits data snooping.

EXAMPLE 3-6

Consider the data in Example 3-1. There are five treatment means and four degrees of freedom between these treatments. Suppose that prior to running the experiment the following set of comparisons among the treatment means (and their associated contrasts) were specified:

Hypothesis	Contrast
$H_0: \mu_4 = \mu_5$	$C_1 = -y_{4.} + y_{5.}$
$H_0: \mu_1 + \mu_3 = \mu_4 + \mu_5$	$C_2 = y_{1.} + y_{3.} - y_{4.} - y_{5.}$
$H_0: \mu_1 = \mu_3$	$C_3 = y_{1.} - y_{3.}$
$H_0: 4\mu_2 = \mu_1 + \mu_3 + \mu_4 + \mu_5$	$C_4 = -y_{1.} + 4y_{2.} - y_{3.} - y_{4.} - y_{5.}$

Notice that the contrast coefficients are orthogonal. Using the data in Table 3-4, we find the numerical values of the contrasts and the sums of squares to be as follows:

$$C_1 = -1(108) + 1(54) = -54 \qquad SS_{C_1} = \frac{(-54)^2}{5(2)} = 291.60$$

$$C_2 = +1(49) + 1(88) - 1(108) - 1(54) = -25 \qquad SS_{C_2} = \frac{(-25)^2}{5(4)} = 31.25$$

$$C_3 = +1(49) - 1(88) = -39 \qquad SS_{C_3} = \frac{(-39)^2}{5(2)} = 152.10$$

$$C_4 = -1(49) + 4(77) - 1(88) - 1(108) - 1(54) = 9 \qquad SS_{C_4} = \frac{(9)^2}{5(20)} = 0.81$$

Table 3-11 Analysis of Variance for the Tensile Strength Data

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Cotton Weight Percentage	475.76	4	118.94	14.76	<0.001
orthogonal contrasts					
$C_1: \mu_4 = \mu_5$	(291.60)	1	291.60	36.18	<0.001
$C_2: \mu_1 + \mu_3 = \mu_4 + \mu_5$	(31.25)	1	31.25	3.88	0.06
$C_3: \mu_1 = \mu_3$	(152.10)	1	152.10	18.87	<0.001
$C_4: 4\mu_2 = \mu_1 + \mu_3 + \mu_4 + \mu_5$	(0.81)	1	0.81	0.10	0.76
Error	161.20	20	8.06		
Total	636.96	24			

These contrast sums of squares completely partition the treatment sum of squares. The tests on such orthogonal contrasts are usually incorporated in the analysis of variance, as shown in Table 3-11. We conclude from the P-values that there are significant differences between levels 4 and 5 and 1 and 3 of cotton weight percent but that the *average* of levels 1 and 3 does not differ from the average of levels 4 and 5 at the $\alpha = 0.05$ level, and that level 2 does not differ from the average of the other four levels.

3-5.6 Scheffé's Method for Comparing All Contrasts

In many situations, experimenters may not know in advance which contrasts they wish to compare, or they may be interested in more than $a - 1$ possible comparisons. In many exploratory experiments, the comparisons of interest are discovered only after preliminary examination of the data. Scheffé (1953) has proposed a method for comparing any and all possible contrasts between treatment means. In the Scheffé method, the type I error is at most α for any of the possible comparisons.

Suppose that a set of m contrasts in the treatment means

$$\Gamma_u = c_{1u}\mu_1 + c_{2u}\mu_2 + \cdots + c_{au}\mu_a \qquad u = 1, 2, \ldots, m \tag{3-31}$$

of interest have been determined. The corresponding contrast in the treatment averages $\bar{y}_{i.}$ is

$$C_u = c_{1u}\bar{y}_{1.} + c_{2u}\bar{y}_{2.} + \cdots + c_{au}\bar{y}_{a.} \qquad u = 1, 2, \ldots, m \tag{3-32}$$

and the **standard error** of this contrast is

$$S_{C_u} = \sqrt{MS_E \sum_{i=1}^{a} (c_{iu}^2/n_i)} \tag{3-33}$$

where n_i is the number of observations in the ith treatment. It can be shown that the critical value against which C_u should be compared is

$$S_{\alpha,u} = S_{C_u}\sqrt{(a-1)F_{\alpha,a-1,N-a}} \tag{3-34}$$

To test the hypothesis that the contrast Γ_u differs significantly from zero, refer C_u to the critical value. If $|C_u| > S_{\alpha,u}$, the hypothesis that the contrast Γ_u equals zero is rejected.

The Scheffé procedure can also be used to form confidence intervals for all possible contrasts among treatment means. The resulting intervals, say $C_u - S_{\alpha,u} \leq \Gamma_u \leq C_u + S_{\alpha,u}$, are **simultaneous confidence intervals** in that the probability is at least $1 - \alpha$ that all of them are simultaneously true.

To illustrate the procedure, consider the data in Example 3-1 and suppose that the contrasts of interests are

$$\Gamma_1 = \mu_1 + \mu_3 - \mu_4 - \mu_5$$

and

$$\Gamma_2 = \mu_1 - \mu_4$$

The numerical values of these contrasts are

$$\begin{aligned} C_1 &= \bar{y}_{1.} + \bar{y}_{3.} - \bar{y}_{4.} - \bar{y}_{5.} \\ &= 9.80 + 17.60 - 21.60 - 10.80 \\ &= 5.00 \end{aligned}$$

and

$$\begin{aligned} C_2 &= \bar{y}_{1.} - \bar{y}_{4.} \\ &= 9.80 - 21.60 \\ &= -11.80 \end{aligned}$$

and the standard errors are found from Equation 3-33 as

$$S_{C_1} = \sqrt{MS_E \sum_{i=1}^{5} (c_{i1}^2/n_i)} = \sqrt{8.06(1 + 1 + 1 + 1)/5)} = 2.54$$

and

$$S_{C_2} = \sqrt{MS_E \sum_{i=1}^{5} (c_{i2}^2/n_i)} = \sqrt{8.06(1 + 1)/5} = 1.80$$

From Equation 3-34, the 1 percent critical values are

$$S_{0.01,1} = S_{C_1}\sqrt{(a - 1)F_{0.01,a-1,N-a}} = 2.54\sqrt{4(4.43)} = 10.69$$

and

$$S_{0.01,2} = S_{C_2}\sqrt{(a - 1)F_{0.01,a-1,N-a}} = 1.80\sqrt{4(4.43)} = 7.58$$

Because $|C_1| < S_{0.01,1}$, we conclude that the contrast $\Gamma_1 = \mu_1 + \mu_3 - \mu_4 - \mu_5$ equals zero; that is, there is no strong evidence to conclude that the means of treatments 1 and 3 as a group differ from the means of treatments 4 and 5 as a group. However, because $|C_2| > S_{0.01,2}$, we conclude that the contrast $\Gamma_2 = \mu_1 - \mu_4$ does not equal zero; that is, the mean strengths of treatments 1 and 4 differ significantly.

In many practical situations, we will wish to compare only **pairs of means**. Frequently, we can determine which means differ by testing the differences between *all* pairs of treatment means. Thus, we are interested in contrasts of the form $\Gamma = \mu_i - \mu_j$ for all $i \neq j$. Although the Scheffé method could be easily applied to this problem, it is not the most sensitive procedure for such comparisons. We now turn to a consideration of methods specifically designed for pairwise comparisons between all a population means.

3-5.7 Comparing Pairs of Treatment Means

Suppose that we are interested in comparing all pairs of a treatment means and that the null hypotheses that we wish to test are $H_0: \mu_i = \mu_j$ for all $i \neq j$. We now present four methods for making such comparisons.

Tukey's Test

Suppose that, following an analysis of variance in which we have rejected the null hypothesis of equal treatment means, we wish to test all pairwise mean comparisons:

$$\begin{aligned} H_0&: \mu_i = \mu_j \\ H_1&: \mu_i \neq \mu_j \end{aligned}$$

for all $i \neq j$. Tukey (1953) proposed a procedure for testing hypotheses for which the overall significance level is exactly α when the sample sizes are equal and at most α

when the sample sizes are unequal. His procedure can also be used to contract confidence intervals on the differences in all pairs of means. For these intervals, the simultaneous confidence level is $100(1 - \alpha)$ percent when the sample sizes are equal and at least $100(1 - \alpha)$ percent when sample sizes are unequal. This is an excellent data snooping procedure when interest focuses on pairs of means.

Tukey's procedure makes use of the distribution of the **studentized range statistic**

$$q = \frac{\bar{y}_{\max} - \bar{y}_{\min}}{\sqrt{MS_E/n}}$$

where $\bar{y}_{\max}$ and $\bar{y}_{\min}$ are the largest and smallest sample means, respectively, out of a group of p sample means. Appendix Table VIII contains values of $q_\alpha(p, f)$, the upper α percentage points of q where f is the number of degrees of freedom associated with the MS_E. For equal sample sizes, Tukey's test declares two means significantly different if the absolute value of their sample differences exceeds

$$T_\alpha = q_\alpha(a, f)\sqrt{\frac{MS_E}{n}} \tag{3-35}$$

Equivalently, we could construct a set of $100(1 - \alpha)$ percent confidence intervals for all pairs of means as follows:

$$\bar{y}_{i.} - \bar{y}_{j.} - q_\alpha(a, f)\sqrt{\frac{MS_E}{n}} \leq \mu_i - \mu_j \leq \bar{y}_{i.} - \bar{y}_{j.} + q_\alpha(a, f)\sqrt{\frac{MS_E}{n}}, \quad i \neq j. \tag{3-36}$$

When sample sizes are not equal, Equations 3-35 and 3-36 become

$$T_\alpha = \frac{q_\alpha(a, f)}{\sqrt{2}}\sqrt{MS_E\left(\frac{1}{n_i} + \frac{1}{n_j}\right)} \tag{3-37}$$

and

$$\bar{y}_{i.} - \bar{y}_{j.} - \frac{q_\alpha(a, f)}{\sqrt{2}}\sqrt{MS_E\left(\frac{1}{n_i} + \frac{1}{n_j}\right)} \leq \mu_i - \mu_j \leq \bar{y}_{i.} - \bar{y}_{j.} + \frac{q_\alpha(a, f)}{\sqrt{2}}\sqrt{MS_E\left(\frac{1}{n_i} + \frac{1}{n_j}\right)}, \; i \neq j \tag{3-38}$$

respectively. The unequal sample size version is sometimes called the **Tukey–Kramer procedure**.

EXAMPLE 3-7

To illustrate Tukey's test, we use the data from the cotton weight percentage experiment in Example 3-1. With $\alpha = 0.05$ and $f = 20$ degrees of freedom for error, Appendix Table VIII gives $q_{0.05}(5, 20) = 4.23$. Therefore, from Equation 3-35,

$$T_{0.05} = q_{0.05}(5, 20)\sqrt{\frac{MS_E}{n}} = 4.23\sqrt{\frac{8.06}{5}} = 5.37$$

$\bar{y}_{1.}$	$\bar{y}_{5.}$	$\bar{y}_{2.}$	$\bar{y}_{3.}$	$\bar{y}_{4.}$
9.8	10.8	15.4	17.6	21.6

Figure 3-12 Results of Tukey's test.

Thus, any pair of treatment averages that differ in absolute value by more than 5.37 would imply that the corresponding pair of population means are significantly different. The five treatment averages are

$$\bar{y}_{1.} = 9.8 \quad \bar{y}_{2.} = 15.4 \quad \bar{y}_{3.} = 17.6 \quad \bar{y}_{4.} = 21.6 \quad \bar{y}_{5.} = 10.8$$

and the differences in averages are

$$\begin{aligned}
\bar{y}_{1.} - \bar{y}_{2.} &= 9.8 - 15.4 = -5.6^* \\
\bar{y}_{1.} - \bar{y}_{3.} &= 9.8 - 17.6 = -7.8^* \\
\bar{y}_{1.} - \bar{y}_{4.} &= 9.8 - 21.6 = -11.8^* \\
\bar{y}_{1.} - \bar{y}_{5.} &= 9.8 - 10.8 = -1.0 \\
\bar{y}_{2.} - \bar{y}_{3.} &= 15.4 - 17.6 = -2.2 \\
\bar{y}_{2.} - \bar{y}_{4.} &= 15.4 - 21.6 = -6.2^* \\
\bar{y}_{2.} - \bar{y}_{5.} &= 15.4 - 10.8 = 4.6 \\
\bar{y}_{3.} - \bar{y}_{4.} &= 17.6 - 21.6 = -4.0 \\
\bar{y}_{3.} - \bar{y}_{5.} &= 17.6 - 10.8 = 6.8^* \\
\bar{y}_{4.} - \bar{y}_{5.} &= 21.6 - 10.8 = 10.8^*
\end{aligned}$$

The starred values indicate pairs of means that are significantly different. It is usually helpful to draw a graph, such as in Figure 3-12, underlining pairs of means that do not differ significantly. This graph gives an indication that the treatment means form three groups: μ_1 and μ_5, μ_2 and μ_3, and μ_4. However, the membership in these groups is not completely distinct.

When using any procedure for pairwise testing of means we occasionally find that the overall F test from the analysis of variance is significant, but the pairwise comparison of means fails to reveal any significant differences. This situation occurs because the F test is simultaneously considering all possible contrasts involving the treatment means, not just pairwise comparisons. That is, in the data at hand, the significant contrasts may not be of the form $\mu_i - \mu_j$.

Some computer software packages present pairwise comparisons with confidence intervals. For the Tukey procedure, these intervals would be computed from either Equation 3-36 or 3-38, depending on whether or not the sample sizes are equal.

The derivation of the Tukey confidence interval of Equation 3-36 for equal sample sizes is straightforward. For the studentized range statistic q we have

$$P\left(\frac{\max(\bar{y}_{i.} - \mu_i) - \min(\bar{y}_{i.} - \mu_i)}{\sqrt{MS_E/n}} \leq q_\alpha(a, f)\right) = 1 - \alpha$$

If $\max(\bar{y}_{i.} - \mu_i) - \min(\bar{y}_{i.} - \mu_i)$ is less than or equal to $q_\alpha(a,f)\sqrt{MS_E/n}$, it must be true that $|(\bar{y}_{i.} - \mu_i) - (\bar{y}_{j.} - \mu_j)| \leq q_\alpha(a,f)\sqrt{MS_E/n}$ for every pair of means. Therefore

$$P\left(-q_\alpha(a,f)\sqrt{\frac{MS_E}{n}} \leq \bar{y}_{i.} - \bar{y}_{j.} - (\mu_i - \mu_j) \leq q_\alpha(a,f)\sqrt{\frac{MS_E}{n}}\right) = 1 - \alpha$$

Rearranging this expression to isolate $\mu_i - \mu_j$ between the inequalities will lead to the set of $100(1 - \alpha)$ percent simultaneous confidence intervals given in Equation 3-38.

The Fisher Least Significant Difference (LSD) Method

This procedure uses the F statistic for testing $H_0: \mu_i = \mu_j$

$$t_0 = \frac{\bar{y}_{i.} - \bar{y}_{j.}}{\sqrt{MS_E\left(\frac{1}{n_i} + \frac{1}{n_j}\right)}} \tag{3-39}$$

Assuming a two-sided alternative, the pair of means μ_i and μ_j would be declared significantly different if $|\bar{y}_{i.} - \bar{y}_{j.}| > t_{\alpha/2,N-a}\sqrt{MS_E(1/n_i + 1/n_j)}$. The quantity

$$\text{LSD} = t_{\alpha/2,N-a}\sqrt{MS_E\left(\frac{1}{n_i} + \frac{1}{n_j}\right)} \tag{3-40}$$

is called the **least significant difference**. If the design is balanced, $n_1 = n_2 = \cdots = n_a = n$, and

$$\text{LSD} = t_{\alpha/2,N-a}\sqrt{\frac{2MS_E}{n}} \tag{3-41}$$

To use the Fisher LSD procedure, we simply compare the observed difference between each pair of averages to the corresponding LSD. If $|\bar{y}_{i.} - \bar{y}_{j.}| > \text{LSD}$, we conclude that the population means μ_i and μ_j differ.

EXAMPLE 3-8

To illustrate the procedure, if we use the data from the experiment in Example 3-1, the LSD at $\alpha = 0.05$ is

$$\text{LSD} = t_{.025,20}\sqrt{\frac{2MS_E}{n}} = 2.086\sqrt{\frac{2(8.06)}{5}} = 3.75$$

Thus, any pair of treatment averages that differ in absolute value by more than 3.75 would imply that the corresponding pair of population means are significantly different. The differences in averages are

$$\begin{aligned}
\bar{y}_{1.} - \bar{y}_{2.} &= 9.8 - 15.4 = -5.6^* \\
\bar{y}_{1.} - \bar{y}_{3.} &= 9.8 - 17.6 = -7.8^* \\
\bar{y}_{1.} - \bar{y}_{4.} &= 9.8 - 21.6 = -11.8^* \\
\bar{y}_{1.} - \bar{y}_{5.} &= 9.8 - 10.8 = -1.0 \\
\bar{y}_{2.} - \bar{y}_{3.} &= 15.4 - 17.6 = -2.2 \\
\bar{y}_{2.} - \bar{y}_{4.} &= 15.4 - 21.6 = -6.2^* \\
\bar{y}_{2.} - \bar{y}_{5.} &= 15.4 - 10.8 = 4.6^* \\
\bar{y}_{3.} - \bar{y}_{4.} &= 17.6 - 21.6 = -4.0^* \\
\bar{y}_{3.} - \bar{y}_{5.} &= 17.6 - 10.8 = 6.8^* \\
\bar{y}_{4.} - \bar{y}_{5.} &= 21.6 - 10.8 = 10.8^*
\end{aligned}$$

$\bar{y}_{1.}$	$\bar{y}_{5.}$	$\bar{y}_{2.}$	$\bar{y}_{3.}$	$\bar{y}_{4.}$
9.8	10.8	15.4	17.6	21.6

Figure 3-13 Results of the LSD procedure.

The starred values indicate pairs of means that are significantly different. Figure 3-13 summarizes the results. Clearly, the only pairs of means that do not differ significantly are 1 and 5 and 2 and 3, and treatment 4 produces a significantly greater tensile strength than the other treatments.

Note that the overall α risk may be considerably inflated using this method. Specifically, as a gets larger, the type I error of the experiment (the ratio of the number of experiments in which at least one type I error is made to the total number of experiments) becomes large.

Duncan's Multiple Range Test

A widely used procedure for comparing all pairs of means is the **multiple range test** developed by Duncan (1955). To apply Duncan's multiple range test for equal sample sizes, the a treatment averages are arranged in ascending order, and the standard error of each average is determined as

$$S_{\bar{y}_{i.}} = \sqrt{\frac{MS_E}{n}} \tag{3-42}$$

For unequal sample sizes, replace n in Equation 3-42 by the harmonic mean n_h of the $\{n_i\}$, where

$$n_h = \frac{a}{\sum_{i=1}^{a} (1/n_i)} \tag{3-43}$$

Note that if $n_1 = n_2 = \cdots = n_a$, $n_h = n$. From Duncan's table of significant ranges (Appendix Table VII), obtain the values $r_\alpha(p, f)$ for $p = 2, 3, \ldots, a$, where α is the significance level and f is the number of degrees of freedom for error. Convert these ranges into a set of $a - 1$ least significant ranges (e.g., R_p) for $p = 2, 3, \ldots, a$ by calculating

$$R_p = r_\alpha(p, f)S_{\bar{y}_{i.}} \qquad \text{for } p = 2, 3, \ldots, a \tag{3-44}$$

Then, the observed differences between means are tested, beginning with largest versus smallest, which would be compared with the least significant range R_a. Next, the difference of the largest and the second-smallest is computed and compared with the least significant range R_{a-1}. These comparisons are continued until all means have been compared with the largest mean. Finally, the difference between the second-largest mean and the smallest is computed and compared against the least significant range R_{a-1}. This process is continued until the differences between all possible $a(a - 1)/2$ pairs of means have been considered. If an observed difference is greater than the corresponding least significant range, we conclude that the pair of means in question is significantly different. To prevent contradictions, no differences between a pair of means are considered sig-

nificant if the two means involved fall between two other means that do not differ significantly.

EXAMPLE 3-9

We can apply Duncan's multiple range test to the experiment of Example 3-1. Recall that $MS_E = 8.06$, $N = 25$, $n = 5$, and there are 20 error degrees of freedom. Ranking the treatment averages in ascending order, we have

$$\bar{y}_{1.} = 9.8$$
$$\bar{y}_{5.} = 10.8$$
$$\bar{y}_{2.} = 15.4$$
$$\bar{y}_{3.} = 17.6$$
$$\bar{y}_{4.} = 21.6$$

The standard error of each average is $S_{\bar{y}_{i.}} = \sqrt{8.06/5} = 1.27$. From the table of significant ranges in Appendix Table VII for 20 degrees of freedom and $\alpha = 0.05$, we obtain $r_{0.05}(2, 20) = 2.95$, $r_{0.05}(3, 20) = 3.10$, $r_{0.05}(4, 20) = 3.18$, and $r_{0.05}(5, 20) = 3.25$. Thus, the least significant ranges are

$$R_2 = r_{0.05}(2, 20)S_{\bar{y}_{i.}} = (2.95)(1.27) = 3.75$$
$$R_3 = r_{0.05}(3, 20)S_{\bar{y}_{i.}} = (3.10)(1.27) = 3.94$$
$$R_4 = r_{0.05}(4, 20)S_{\bar{y}_{i.}} = (3.18)(1.27) = 4.04$$
$$R_5 = r_{0.05}(5, 20)S_{\bar{y}_{i.}} = (3.25)(1.27) = 4.13$$

The comparisons would yield

$$4 \text{ vs. } 1: 21.6 - 9.8 = 11.8 > 4.13(R_5)$$
$$4 \text{ vs. } 5: 21.6 - 10.8 = 10.8 > 4.04(R_4)$$
$$4 \text{ vs. } 2: 21.6 - 15.4 = 6.2 > 3.94(R_3)$$
$$4 \text{ vs. } 3: 21.6 - 17.6 = 4.0 > 3.75(R_2)$$
$$3 \text{ vs. } 1: 17.6 - 9.8 = 7.8 > 4.04(R_4)$$
$$3 \text{ vs. } 5: 17.6 - 10.8 = 6.8 > 3.95(R_3)$$
$$3 \text{ vs. } 2: 17.6 - 15.4 = 2.2 < 3.75(R_2)$$
$$2 \text{ vs. } 1: 15.4 - 9.8 = 5.6 > 3.94(R_3)$$
$$2 \text{ vs. } 5: 15.4 - 10.8 = 4.6 > 3.75(R_2)$$
$$5 \text{ vs. } 1: 10.8 - 9.8 = 1.0 < 3.75(R_2)$$

From the analysis we see that there are significant differences between all pairs of means except 3 and 2 and 5 and 1. A graph underlying those means that are not significantly different is shown in Figure 3-14. Notice that, in this example, Duncan's multiple range test and the LSD method produce identical conclusions.

$\bar{y}_{1.}$	$\bar{y}_{5.}$	$\bar{y}_{2.}$	$\bar{y}_{3.}$	$\bar{y}_{4.}$
9.8	10.8	15.4	17.6	21.6

Figure 3-14 Results of Duncan's multiple range test.

Duncan's test requires a greater observed difference to detect significantly different pairs of means as the number of means included in the group increases. For instance, in the above example $R_2 = 3.75$ (two means) whereas $R_3 = 3.94$ (three means). For two means, the critical value R_2 will always exactly equal the LSD value from the t test. The values $r_\alpha(p, f)$ in Appendix Table VII are chosen so that a specified **protection level** is obtained. That is, when two means that are p steps apart are compared, the protection level is $(1 - \alpha)^{p-1}$, where α is the level of significance specified for two *adjacent* means. Thus, the error rate is $1 - (1 - \alpha)^{p-1}$ of reporting at least one incorrect significant difference between two means when the group size is p. For example, if $\alpha = 0.05$, then $1 - (1 - 0.05)^1 = 0.05$ is the significance level for comparing the adjacent pair of means, $1 - (1 - 0.05)^2 = .10$ is the significance level for means that are one step apart, and so forth.

Generally, if the protection level is α, tests on means have a significance level that is greater than or equal to α. Consequently, Duncan's procedure is quite powerful; that is, it is very effective at detecting differences between means when real differences exist. For this reason, Duncan's multiple range test is very popular.

The Newman-Keuls Test

This test was devised by Newman (1939). Because new interest in Newman's test was generated by Keuls (1952), the procedure is usually called the Newman-Keuls test. Operationally, the procedure is similar to Duncan's multiple range test, except that the critical differences between means are calculated somewhat differently. Specifically, we compute a set of critical values

$$K_p = q_\alpha(p, f)S_{\bar{y}_{i.}} \qquad p = 2, 3, \ldots, a \tag{3-45}$$

where $q_\alpha(p, f)$ is the upper α percentage point of the studentized range for groups of means of size p and f error degrees of freedom. Once the values K_p are computed from Equation 3-45, extreme pairs of means in groups of size p are compared with K_p exactly as in Duncan's multiple range test.

Which Pairwise Comparison Method Do I Use?

Certainly a logical question at this point is Which one of these procedures should I use? Unfortunately, there is no clear-cut answer to this question, and professional statisticians often disagree over the utility of the various procedures. Carmer and Swanson (1973) have conducted Monte Carlo simulation studies of a number of multiple comparison procedures, including others not discussed here. They report that the least significant difference method is a very effective test for detecting true differences in means if it is applied *only after* the F test in the analysis of variance is significant at 5 percent. They also report good performance in detecting true differences with Duncan's multiple range test. This is not surprising, because these two methods are the most powerful of those we have discussed. However, these methods do not contain the experimentwise error rate. Because the Tukey method does control the overall error rate, many statisticians prefer to use it.

The Newman–Keuls test is more conservative than Duncan's test in that the type I error rate is smaller. Specifically, the type I error of the experiment is α for all tests involving the same number of means. Consequently, because α is generally lower, the power of the Newman–Keuls test is generally less than that of Duncan's test. To demonstrate that the Newman–Keuls procedure leads to a less powerful test than Duncan's multiple range test, we note from a comparison of Tables VII and VIII of the Appendix that for $p > 2$ we have $q_\alpha(p, f) > r_\alpha(p, f)$. That is, it is "harder" to declare a pair of

means significantly different using the Newman–Keuls test than it is using Duncan's procedure. This is illustrated below for the case $\alpha = 0.01$, $a = 8$, and $f = 20$:

p	2	3	4	5	6	7	8
$r_{0.01}(p, 20)$	4.02	4.22	4.33	4.40	4.47	4.53	4.58
$q_{0.01}(p, 20)$	4.02	4.64	5.02	5.29	5.51	5.69	5.84

As indicated above, there are several other multiple comparison procedures. For articles describing these methods, see Miller (1977), O'Neill and Wetherill (1971), and Nelson (1989). The book by Miller (1991) is also recommended.

3-5.8 Comparing Treatment Means with a Control

In many experiments, one of the treatments is a **control**, and the analyst is interested in comparing each of the other $a - 1$ treatment means with the control. Thus, there are only $a - 1$ comparisons to be made. A procedure for making these comparisons has been developed by Dunnett (1964). Suppose that treatment a is the control and we wish to test the hypotheses

$$H_0: \mu_i = \mu_a$$
$$H_1: \mu_i \neq \mu_a$$

for $i = 1, 2, \ldots, a - 1$. Dunnett's procedure is a modification of the usual t-test. For each hypothesis, we compute the observed differences in the sample means

$$|\bar{y}_{i.} - \bar{y}_{a.}| \qquad i = 1, 2, \ldots, a - 1$$

The null hypothesis $H_0: \mu_i = \mu_a$ is rejected using a type I error rate α if

$$|\bar{y}_{i.} - \bar{y}_{a.}| > d_\alpha(a - 1, f)\sqrt{MS_E\left(\frac{1}{n_i} + \frac{1}{n_a}\right)} \tag{3-46}$$

where the constant $d_\alpha(a - 1, f)$ is given in Appendix Table IX. (Both two- and one-sided tests are possible.) Note that α is the **joint significance level** associated with all $a - 1$ tests.

EXAMPLE 3-10

To illustrate Dunnett's test, consider the experiment from Example 3-1 with treatment 5 considered the control. In this example, $a = 5$, $a - 1 = 4$, $f = 20$, and $n_i = n = 5$. At the 5 percent level, we find from Appendix Table IX that $d_{0.05}(4, 20) = 2.65$. Thus, the critical difference becomes

$$d_{0.05}(4, 20)\sqrt{\frac{2MS_E}{n}} = 2.65\sqrt{\frac{2(8.06)}{5}} = 4.76$$

(Note that this is a simplification of Equation 3-46 resulting from a balanced design.) Thus, any treatment mean that differs from the control by more than 4.76 would be declared significantly different. The observed differences are

$$1 \text{ vs. } 5: \bar{y}_{1.} - \bar{y}_{5.} = 9.8 - 10.8 = -1.0$$
$$2 \text{ vs. } 5: \bar{y}_{2.} - \bar{y}_{5.} = 15.4 - 10.8 = 4.6$$
$$3 \text{ vs. } 5: \bar{y}_{3.} - \bar{y}_{5.} = 17.6 - 10.8 = 6.8$$
$$4 \text{ vs. } 5: \bar{y}_{4.} - \bar{y}_{5.} = 21.6 - 10.8 = 10.8$$

Only the differences $\bar{y}_{3.} - \bar{y}_{5.}$ and $\bar{y}_{4.} - \bar{y}_{5.}$ indicate any significant difference when compared to the control; thus, we conclude that $\mu_3 \neq \mu_5$ and $\mu_4 \neq \mu_5$.

When comparing treatments with a control, it is a good idea to use more observations for the control treatment (say n_a) than for the other treatments (say n), assuming equal numbers of observations for the remaining $a - 1$ treatments. The ratio n_a/n should be chosen to be approximately equal to the square root of the total number of treatments. That is, choose $n_a/n = \sqrt{a}$.

3-6 SAMPLE COMPUTER OUTPUT

Computer programs for supporting experimental design and performing the analysis of variance are widely available. The output from one such program, Design-Expert, is shown in Figure 3-15 (on the facing page), using the data from the single-factor experiment in Example 3-1. The sum of squares corresponding to the "Model" is the usual $SS_{\text{Treatments}}$ for a single-factor design. That source is further identified as "*A*." When there is more than one factor in the experiment, the model sum of squares will be decomposed into several sources (*A*, *B*, etc.). Notice that the analysis of variance summary at the top of the computer output contains the usual sums of squares, degrees of freedom, mean squares, and test statistic F_0. The column "Prob > F" is the *P*-value (actually, the upper bound on the *P*-value, because probabilities less than 0.0001 are defaulted to 0.0001).

In addition to the basic analysis of variance, the program displays some additional useful information. The quantity "R-squared" is defined as

$$R^2 = \frac{SS_{\text{Model}}}{SS_{\text{Total}}} = \frac{475.76}{636.96} = 0.746923$$

and is loosely interpreted as the proportion of the variability in the data "explained" by the analysis of variance model. Thus, in the synthetic fiber strength testing data, the factor "cotton weight percentage" explains about 74.69 percent of the variability in tensile strength. Clearly, we must have $0 \leq R^2 \leq 1$, with larger values being more desirable. There are also some other R^2-like statistics displayed in the output. The "adjusted" R^2 is a variation of the ordinary R^2 statistic that reflects the number of factors in the model. It can be a useful statistic for more complex experiments with several design factors when we wish to evaluate the impact of increasing or decreasing the number of model terms. "Std.Dev." is the square root of the error mean square, $\sqrt{8.060} = 2.839$, and "C.V." is the coefficient of variation, defined as $(\sqrt{MS_E}/\bar{y})100$. The coefficient of variation measures the unexplained or residual variability in the data as a percentage of the mean of the response variable. "PRESS" stands for "Prediction Error Sum of Squares," and it is a measure of how well the model for the experiment is likely to predict the responses in a *new experiment*. Small values of PRESS are desirable. Alternatively, one can calculate an R^2 for predictions based on PRESS (we will show how to do this later). This R^2_{Pred} in our problem is 0.6046, which is not unreasonable, considering that the model accounts for about 75 percent of the variability in the current experiment. The "Adequate Precision" statistic is computed by dividing the difference between the maximum predicted response and the minimum predicted response by the average standard deviation of all predicted responses. Large values of this quantity are desirable, and

Use your mouse to right click on individual cells for definitions.

Response: Strength in psi
ANOVA for Selected Factorial Model
Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Model	475.76	4	118.94	14.76	<0.0001	significant
A	*475.76*	*4*	*118.94*	*14.76*	*<0.0001*	
Residual	161.20	20	8.06			
Lack of Fit	*0.000*	*0*				
Pure Error	*161.20*	*20*	*8.06*			
Cor Total	636.96	24				

The Model F-value of 14.76 implies the model is significant. There is only a 0.01% chance that a "Model F-Value" this large could occur due to noise.

Values of "Prob > F" less than 0.0500 indicate model terms are significant.
In this case A are significant model terms.
Values greater than 0.1000 indicate the model terms are not significant.
If there are many insignificant model terms (not counting those required to support hierarchy), model reduction may improve your model.

Std. Dev.	2.84	R-Squared	0.7469
Mean	15.04	Adj R-Squared	0.6963
C.V.	18.88	Pred R-Squared	0.6046
PRESS	251.88	Adeq Precision	9.294

The "Pred R-Squared" of 0.6046 is in reasonable agreement with the "Adj R-Squared" of 0.6963. A difference greater than 0.20 between the "Pred R-Squared" and the "Adj R-Squared" indicates a possible problem with your model and/or data.

"Adeq Precision" measures the signal to noise ratio. A ratio greater than 4 is desirable. Your ratio of 9.294 indicates an adequate signal to use this model to navigate the design space.

Treatment Means (Adjusted, If Necessary)

	Estimated Mean	Standard Error
1-15	9.80	1.27
2-20	15.40	1.27
3-25	17.60	1.27
4-30	21.60	1.27
5-35	10.80	1.27

Treatment	Mean Difference	DF	Standard Error	t for H_0 Coeff=0	Prob > |t|
1 vs 2	−5.60	1	1.80	−3.12	0.0054
1 vs 3	−7.80	1	1.80	−4.34	0.0003
1 vs 4	−11.80	1	1.80	−6.57	<0.0001
1 vs 5	−1.00	1	1.80	−0.56	0.5838
2 vs 3	−2.20	1	1.80	−1.23	0.2347
2 vs 4	−6.20	1	1.80	−3.45	0.0025
2 vs 5	4.60	1	1.80	2.56	0.0186
3 vs 4	−4.00	1	1.80	−2.23	0.0375
3 vs 5	6.80	1	1.80	3.79	0.0012
4 vs 5	10.80	1	1.80	6.01	<0.0001

Values of "Prob > |t|" less than 0.0500 indicate the difference in the two treatment means is significant.
Values of "Prob > |t|" greater than 0.1000 indicate the difference in the two treatment means is not significant.

Figure 3-15 Design-Expert computer output for Example 3-1.

Diagnostic Case Statistics

Standard Order	Actual Value	Predicted Value	Residual	Leverage	Student Residual	Cook's Distance	Outlier t
1	7.00	9.80	−2.80	0.200	−1.103	0.061	−1.109
2	7.00	9.80	−2.80	0.200	−1.103	0.061	−1.109
3	15.00	9.80	5.20	0.200	2.048	0.210	2.245
4	11.00	9.80	1.20	0.200	0.473	0.011	0.463
5	9.00	9.80	−0.80	0.200	−0.315	0.005	−0.308
6	12.00	15.40	−3.40	0.200	−1.339	0.090	−1.368
7	17.00	15.40	1.60	0.200	0.630	0.020	0.620
8	12.00	15.40	−3.40	0.200	−1.339	0.090	−1.368
9	18.00	15.40	2.60	0.200	1.024	0.052	1.025
10	18.00	15.40	2.60	0.200	1.024	0.052	1.025
11	14.00	17.60	−3.60	0.200	−1.418	0.100	−1.457
12	18.00	17.60	0.40	0.200	0.158	0.001	0.154
13	18.00	17.60	0.40	0.200	0.158	0.001	0.154
14	19.00	17.60	1.40	0.200	0.551	0.015	0.542
15	19.00	17.60	1.40	0.200	0.551	0.015	0.542
16	19.00	21.60	−2.60	0.200	−1.024	0.052	−1.025
17	25.00	21.60	3.40	0.200	1.339	0.090	1.368
18	22.00	21.60	0.40	0.200	0.158	0.001	0.154
19	19.00	21.60	−2.60	0.200	−1.024	0.052	−1.025
20	23.00	21.60	1.40	0.200	0.551	0.015	0.542
21	7.00	10.80	−3.80	0.200	−1.496	0.112	−1.548
22	10.00	10.80	−0.80	0.200	−0.315	0.005	−0.308
23	11.00	10.80	0.20	0.200	0.079	0.000	0.077
24	15.00	10.80	4.20	0.200	1.654	0.137	1.735
25	11.00	10.80	0.20	0.200	0.079	0.000	0.077

Proceed to Diagnostic Plots (the next icon in progression). Be sure to look at the:
1) Normal probability plot of the studentized residuals to check for normality of residuals.
2) Studentized residuals versus predicted values to check for constant error.
3) Outlier t versus run order to look for outliers, i.e., influential values.
4) Box-Cox plot for power transformations.

If all the model statistics and diagnostic plots are OK, finish up with the Model Graphs icon.

Figure 3-15 *(Continued)*

values that exceed four usually indicate that the model will give reasonable performance in prediction.

Treatment means are estimated and the standard error (or sample standard deviation of each treatment mean, $\sqrt{MS_E/n}$) is displayed. Differences between pairs of treatment means are investigated by using the Fisher LSD method described in Section 3-5.7.

The computer program also calculates and displays the residuals, as defined in Equation 3-16. The program will also produce all of the residual plots that we discussed in Section 3-4. There are also several other residual diagnostics displayed in the output. Some of these will be discussed later.

Finally, notice that the computer program also has some interpretative guidance embedded in the output. This "advisory" information is fairly standard in many PC-based statistics packages. Remember in reading such guidance that it is written in very general terms and may not exactly suit the report writing requirements of any specific experimenter. This advisory output may be deleted by the user.

3-7 DETERMINING SAMPLE SIZE

In any experimental design problem, a critical decision is the choice of sample size—that is, determining the number of replicates to run. Generally, if the experimenter is interested in detecting small effects, more replicates are required than if the experimenter is interested in detecting large effects. In this section, we discuss several approaches to determining sample size. Although our discussion focuses on a single-factor design, most of the methods can be used in more complex experimental situations.

3-7.1 Operating Characteristic Curves

Recall that an **operating characteristic curve** is a plot of the type II error probability of a statistical test for a particular sample size versus a parameter that reflects the extent to which the null hypothesis is false. These curves can be used to guide the experimenter in selecting the number of replicates so that the design will be sensitive to important potential differences in the treatments.

We consider the probability of type II error of the fixed effects model for the case of equal sample sizes per treatment, say

$$\begin{aligned}\beta &= 1 - P\{\text{Reject } H_0 | H_0 \text{ is false}\} \\ &= 1 - P\{F_0 > F_{\alpha,a-1,N-a} | H_0 \text{ is false}\}\end{aligned} \tag{3-47}$$

To evaluate the probability statement in Equation 3-47, we need to know the distribution of the test statistic F_0 if the null hypothesis is false. It can be shown that, if H_0 is false, the statistic $F_0 = MS_{\text{Treatments}}/MS_E$ is distributed as a **noncentral F** random variable with $a - 1$ and $N - a$ degrees of freedom and the noncentrality parameter δ. If $\delta = 0$, the noncentral F distribution becomes the usual (central) F distribution.

Operating characteristic curves given in Chart V of the Appendix are used to evaluate the probability statement in Equation 3-47. These curves plot the probability of type II error (β) against a parameter Φ, where

$$\Phi^2 = \frac{n\sum_{i=1}^{a}\tau_i^2}{a\sigma^2} \tag{3-48}$$

The quantity Φ^2 is related to the noncentrality parameter δ. Curves are available for $\alpha = 0.05$ and $\alpha = 0.01$ and a range of degrees of freedom for numerator and denominator.

In using the operating characteristic curves, the experimenter must specify the parameter Φ. This is often difficult to do in practice. One way to determine Φ is to choose the actual values of the treatment means for which we would like to reject the null hypothesis with high probability. Thus, if $\mu_1, \mu_2, \ldots, \mu_a$ are the specified treatment means, we find the τ_i in Equation 3-48 as $\tau_i = \mu_i - \bar{\mu}$, where $\bar{\mu} = (1/a)\sum_{i=1}^{a}\mu_i$ is the average of the individual treatment means. We also require an estimate of σ^2. Sometimes this is available from prior experience, a previous experiment or a preliminary test (as suggested in Chapter 1), or a judgment estimate. When we are uncertain about the value of σ^2, sample sizes could be determined for a range of likely values of σ^2 to study the effect of this parameter on the required sample size before a final choice is made.

EXAMPLE 3-11

Consider the tensile strength experiment described in Example 3-1. Suppose that the experimenter is interested in rejecting the null hypothesis with a probability of at least 0.90 if the five treatment means are

$$\mu_1 = 11 \qquad \mu_2 = 12 \qquad \mu_3 = 15 \qquad \mu_4 = 18 \qquad \text{and} \qquad \mu_5 = 19$$

She plans to use $\alpha = 0.01$. In this case, because $\sum_{i=1}^{5}\mu_i = 75$, we have $\overline{\mu} = (1/5)75 = 15$ and

$$\begin{aligned}
\tau_1 &= \mu_1 - \overline{\mu} = 11 - 15 = -4 \\
\tau_2 &= \mu_2 - \overline{\mu} = 12 - 15 = -3 \\
\tau_3 &= \mu_3 - \overline{\mu} = 15 - 15 = 0 \\
\tau_4 &= \mu_4 - \overline{\mu} = 18 - 15 = 3 \\
\tau_5 &= \mu_5 - \overline{\mu} = 19 - 15 = 4
\end{aligned}$$

Thus, $\sum_{i=1}^{5}\tau_i^2 = 50$. Suppose the experimenter feels that the standard deviation of tensile strength at any particular level of cotton weight percentage will be no larger than $\sigma = 3$ psi. Then, by using Equation 3-48, we have

$$\Phi^2 = \frac{n\sum_{i=1}^{5}\tau_i^2}{a\sigma^2} = \frac{n(50)}{5(3)^2} = 1.11n$$

We use the operating characteristic curve for $a - 1 = 5 - 1 = 4$ with $N - a = a(n - 1) = 5(n - 1)$ error degrees of freedom and $\alpha = 0.01$ (see Appendix Chart V). As a first guess at the required sample size, try $n = 4$ replicates. This yields $\Phi^2 = 1.11(4) = 4.44$, $\Phi = 2.11$, and $5(3) = 15$ error degrees of freedom. Consequently, from Chart V, we find that $\beta \simeq 0.30$. Therefore, the power of the test is approximately $1 - \beta = 1 - 0.30 = 0.70$, which is less than the required 0.90, and so we conclude that $n = 4$ replicates are not sufficient. Proceeding in a similar manner, we can construct the following display:

n	Φ^2	Φ	$a(n-1)$	β	Power $(1-\beta)$
4	4.44	2.11	15	0.30	0.70
5	5.55	2.36	20	0.15	0.85
6	6.66	2.58	25	0.04	0.96

Thus, at least $n = 6$ replicates must be run to obtain a test with the required power.

The only problem with this approach to using the operating characteristic curves is that it is usually difficult to select a set of treatment means on which the sample size decision should be based. An alternate approach is to select a sample size such that if the difference between any two treatment means exceeds a specified value the null hypothesis should be rejected. If the difference between any two treatment means is as large as D, it can be shown that the minimum value of Φ^2 is

$$\Phi^2 = \frac{nD^2}{2a\sigma^2} \tag{3-49}$$

Because this is a minimum value of Φ^2, the corresponding sample size obtained from the operating characteristic curve is a conservative value; that is, it provides a power at least as great as that specified by the experimenter.

To illustrate this approach, suppose that in the tensile strength experiment from Example 3-1, the experimenter wished to reject the null hypothesis with probability at least 0.90 if any two treatment means differed by as much as 10 psi. Then, assuming that $\sigma = 3$ psi, we find the minimum value of Φ^2 to be

$$\Phi^2 = \frac{n(10)^2}{2(5)(3^2)} = 1.11n$$

and, from the analysis in Example 3-11, we conclude that $n = 6$ replicates are required to give the desired sensitivity when $\alpha = 0.01$.

3-7.2 Specifying a Standard Deviation Increase

This approach is occasionally helpful in choosing the sample size. If the treatment means do not differ, the standard deviation of an observation chosen at random is σ. If the treatment means are different, however, the standard deviation of a randomly chosen observation is

$$\sqrt{\sigma^2 + \left(\sum_{i=1}^{a} \tau_i^2/a\right)}$$

If we choose a percentage P for the increase in the standard deviation of an observation beyond which we wish to reject the hypothesis that all treatment means are equal, this is equivalent to choosing

$$\frac{\sqrt{\sigma^2 + \left(\sum_{i=1}^{a} \tau_i^2/a\right)}}{\sigma} = 1 + 0.01P \quad (P = \text{percent})$$

or

$$\frac{\sqrt{\sum_{i=1}^{a} \tau_i^2/a}}{\sigma} = \sqrt{(1 + 0.01P)^2 - 1}$$

so that

$$\Phi = \frac{\sqrt{\sum_{i=1}^{a} \tau_i^2/a}}{\sigma/\sqrt{n}} = \sqrt{(1 + 0.01P)^2 - 1}(\sqrt{n}) \tag{3-50}$$

Thus, for a specified value of P, we may compute Φ from Equation 3-50 and then use the operating characteristic curves in Appendix Chart V to determine the required sample size.

For example, in the tensile strength experiment from Example 3-1, suppose that we wish to detect a standard deviation increase of 20 percent with a probability of at least 0.90 and $\alpha = 0.05$. Then

$$\Phi = \sqrt{(1.2)^2 - 1}(\sqrt{n}) = 0.66\sqrt{n}$$

Reference to the operating characteristic curves shows that $n = 9$ is required to give the desired sensitivity.

3-7.3 Confidence Interval Estimation Method

This approach assumes that the experimenter wishes to express the final results in terms of confidence intervals and is willing to specify in advance how wide he or she wants these confidence intervals to be. For example, suppose that in the tensile strength experiment from Example 3-1 we wanted a 95 percent confidence interval on the difference in mean tensile strength for any two cotton weight percentages to be ± 5 psi and a prior estimate of σ is 3. Then, using Equation 3-13, we find that the accuracy of the confidence interval is

$$\pm t_{\alpha/2,N-a}\sqrt{\frac{2MS_E}{n}}$$

Suppose that we try $n = 5$ replicates. Then, using $\sigma^2 = 3^2 = 9$ as an estimate of MS_E, the accuracy of the confidence interval becomes

$$\pm 2.086\sqrt{\frac{2(9)}{5}} = \pm 3.96$$

which is more accurate than the requirement. Trying $n = 4$ gives

$$\pm 2.132\sqrt{\frac{2(9)}{4}} = \pm 4.52$$

Trying $n = 3$ gives

$$\pm 2.228\sqrt{\frac{2(9)}{3}} = \pm 5.46$$

Clearly $n = 4$ is the smallest sample size that will lead to the desired accuracy.

The quoted level of significance in the above illustration applies only to one confidence interval. However, the same general approach can be used if the experimenter wishes to prespecify a *set* of confidence intervals about which a **joint** or **simultaneous confidence statement** is made (see the comments about simultaneous confidence intervals in Section 3-3.3). Furthermore, the confidence intervals could be constructed about more general contrasts in the treatment means than the pairwise comparison illustrated above.

3-8 DISCOVERING DISPERSION EFFECTS

We have focused on using the analysis of variance and related methods to determine which factor levels result in differences among treatment or factor level means. It is customary to refer to these effects as **location effects**. If there was inequality of variance

Table 3-12 Data for the Smelting Experiment

Ratio Control Algorithm	Observations					
	1	2	3	4	5	6
1	4.93(0.05)	4.86(0.04)	4.75(0.05)	4.95(0.06)	4.79(0.03)	4.88(0.05)
2	4.85(0.04)	4.91(0.02)	4.79(0.03)	4.85(0.05)	4.75(0.03)	4.85(0.02)
3	4.83(0.09)	4.88(0.13)	4.90(0.11)	4.75(0.15)	4.82(0.08)	4.90(0.12)
4	4.89(0.03)	4.77(0.04)	4.94(0.05)	4.86(0.05)	4.79(0.03)	4.76(0.02)

at the different factor levels, we used transformations to stabilize the variance to improve our inference on the location effects. In some problems, however, we are interested in discovering whether the different factor levels affect **variability**; that is, we are interested in discovering potential **dispersion effects**. This will occur whenever the standard deviation, variance, or some other measure of variability is used as a response variable.

To illustrate these ideas, consider the data in Table 3-12, which resulted from a designed experiment in an aluminum smelter. Aluminum is produced by combining alumina with other ingredients in a reaction cell and applying heat by passing electric current through the cell. Alumina is added continuously to the cell to maintain the proper ratio of alumina to other ingredients. Four different ratio control algorithms were investigated in this experiment. The response variables studied were related to cell voltage. Specifically, a sensor scans cell voltage several times each second, producing thousands of voltage measurements during each run of the experiment. The process engineers decided to use the average voltage and the standard deviation of cell voltage (shown in parentheses) over the run as the response variables. The average voltage is important because it affects cell temperature, and the standard deviation of voltage (called "pot noise" by the process engineers) is important because it affects the overall cell efficiency.

An analysis of variance was performed to determine if the different ratio control algorithms affect average cell voltage. This revealed that the ratio control algorithm had no **location effect**; that is, changing the ratio control algorithms does not change the average cell voltage. (Refer to Problem 3-28.)

To investigate dispersion effects, it is usually best to use

$$\log(s) \quad \text{or} \quad \log(s^2)$$

as a response variable since the log transformation is effective in stabilizing variability in the distribution of the sample standard deviation. Because all sample standard deviations of pot voltage are less than unity, we will use

$$y = -\ln(s)$$

as the response variable. Table 3-13 presents the analysis of variance for this response, the natural logarithm of "pot noise'." Notice that the choice of a ratio control algorithm

Table 3-13 Analysis of Variance for the Natural Logarithm of Pot Noise

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Ratio Control Algorithm	6.166	3	2.055	21.96	<0.001
Error	1.872	20	0.094		
Total	8.038	23			

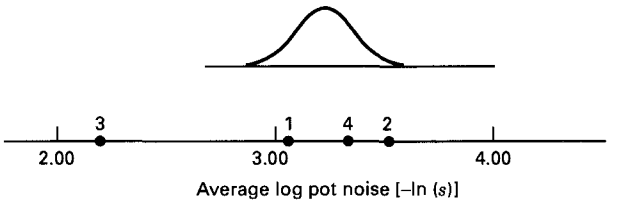


Figure 3-16 Average log pot noise $[-\ln(s)]$ for four ratio control algorithms relative to a scaled t distribution with scale factor $\sqrt{MS_E/n} = \sqrt{0.094/6} = 0.125$.

affects pot noise; that is, the ratio control algorithm has a **dispersion effect**. Standard tests of model adequacy, including normal probability plots of the residuals, indicate that there are no problems with experimental validity. (Refer to Problem 3-29.)

Figure 3-16 plots the average log pot noise for each ratio control algorithm and also presents a scaled t distribution for use as a **reference distribution** in discriminating between ratio control algorithms. This plot clearly reveals that ratio control algorithm 3 produces greater pot noise or greater cell voltage standard deviation than the other algorithms. There does not seem to be much difference between algorithms 1, 2, and 4.

3-9 THE REGRESSION APPROACH TO THE ANALYSIS OF VARIANCE

We have given an intuitive of heuristic development of the analysis of variance. However, it is possible to give a more formal development. The method will be useful later in understanding the basis for the statistical analysis of more complex designs. Called the **general regression significance test**, the procedure essentially consists of finding the reduction in the total sum of squares for fitting the model with all parameters included and the reduction in sum of squares when the model is restricted to the null hypotheses. The difference between these two sums of squares is the treatment sum of squares with which a test of the null hypothesis can be conducted. The procedure requires the least squares estimators of the parameters in the analysis of variance model. We have given these parameter estimates previously (in Section 3-3.3); however, we now give a formal development.

3-9.1 Least Squares Estimation of the Model Parameters

We now develop estimators for the parameter in the single-factor model

$$y_{ij} = \mu + \tau_i + \epsilon_{ij}$$

using the method of least squares. To find the least squares estimators of μ and τ_i, we first form the sum of squares of the errors

$$L = \sum_{i=1}^{a}\sum_{j=1}^{n} \epsilon_{ij}^2 = \sum_{i=1}^{a}\sum_{j=1}^{n} (y_{ij} - \mu - \tau_i)^2 \tag{3-51}$$

and then choose values of μ and τ_i, say $\hat{\mu}$ and $\hat{\tau}_i$, that minimize L. The appropriate values would be the solutions to the $a + 1$ simultaneous equations

$$\left.\frac{\partial L}{\partial \mu}\right|_{\hat{\mu},\hat{\tau}_i} = 0$$

$$\left.\frac{\partial L}{\partial \tau_i}\right|_{\hat{\mu},\hat{\tau}_i} = 0 \qquad i = 1, 2, \ldots, a$$

Differentiating Equation 3-51 with respect to μ and τ_i and equating to zero, we obtain

$$-2 \sum_{i=1}^{a} \sum_{j=1}^{n} (y_{ij} - \hat{\mu} - \hat{\tau}_i) = 0$$

and

$$-2 \sum_{j=1}^{n} (y_{ij} - \hat{\mu} - \hat{\tau}_i) = 0 \qquad i = 1, 2, \ldots, a$$

which, after simplification, yield

$$\begin{aligned} N\hat{\mu} + n\hat{\tau}_1 + n\hat{\tau}_2 + \cdots + n\hat{\tau}_a &= y_{..} \\ n\hat{\mu} + n\hat{\tau}_1 &= y_{1.} \\ n\hat{\mu} + n\hat{\tau}_2 &= y_{2.} \\ &\vdots \quad\quad \vdots \\ n\hat{\mu} + n\hat{\tau}_a &= y_{a.} \end{aligned} \tag{3-52}$$

The $a + 1$ equations (Equation 3-52) in $a + 1$ unknowns are called the **least squares normal equations**. Notice that if we add the last a normal equations, we obtain the first normal equation. Therefore, the normal equations are not linearly independent, and no unique solution for μ, $\tau_1, \ldots, \tau_a$ exists. This difficulty can be overcome by several methods. Because we have defined the treatment effects as deviations from the overall mean, it seems reasonable to apply the **constraint**

$$\sum_{i=1}^{a} \hat{\tau}_i = 0 \tag{3-53}$$

Using this constraint, we obtain as the solution to the normal equations

$$\begin{aligned} \hat{\mu} &= \bar{y}_{..} \\ \hat{\tau}_i &= \bar{y}_{i.} - \bar{y}_{..} \qquad i = 1, 2, \ldots, a \end{aligned} \tag{3-54}$$

This solution is obviously not unique and depends on the constraint (Equation 3-53) that we have chosen. At first this may seem unfortunate because two different experimenters could analyze the same data and obtain different results if they apply different constraints. However, certain **functions** of the model parameter *are* uniquely estimated, regardless of the constraint. Some examples are $\tau_i - \tau_j$, which would be estimated by $\hat{\tau}_i - \hat{\tau}_j = \bar{y}_{i.} - \bar{y}_{j.}$, and the ith treatment mean $\mu_i = \mu + \tau_i$, which would be estimated by $\hat{\mu}_i = \hat{\mu} + \hat{\tau}_i = \bar{y}_{i.}$.

Because we are usually interested in differences among the treatment effects rather than their actual values, it causes no concern that the τ_i cannot be uniquely estimated. In

general, any function of the model parameters that is a linear combination of the left-hand side of the normal equations (Equations 3-52) can be uniquely estimated. Functions that are uniquely estimated regardless of which constraint is used are called **estimable functions**. For more information, see the supplemental material for this chapter. We are now ready to use these parameter estimates in a general development of the analysis of variance.

3-9.2 The General Regression Significance Test

A fundamental part of this procedure is writing the normal equations for the model. These equations may always be obtained by forming the least squares function and differentiating it with respect to each unknown parameter, as we did in Section 3-9.1. However, an easier method is available. The following rules allow the normal equations for *any* experimental design model to be written directly:

RULE 1. There is one normal equation for each parameter in the model to be estimated.

RULE 2. The right-hand side of any normal equation is just the sum of all observations that contain the parameter associated with that particular normal equation.

To illustrate this rule, consider the single-factor model. The first normal equation is for the parameter μ; therefore, the right-hand side is $y_{..}$ because *all* observations contain μ.

RULE 3. The left-hand side of any normal equation is the sum of all model parameters, where each parameter is multiplied by the number of times it appears in the total on the right-hand side. The parameters are written with a circumflex (^) to indicate that they are *estimators* and not the true parameter values.

For example, consider the first normal equation in a single-factor experiment. According to the above rules, it would be

$$N\hat{\mu} + n\hat{\tau}_1 + n\hat{\tau}_2 + \cdots + n\hat{\tau}_a = y_{..}$$

because μ appears in all N observations, τ_1 appears only in the n observations taken under the first treatment, τ_2 appears only in the n observations taken under the second treatment, and so on. From Equation 3-52, we verify that the equation shown above is correct. The second normal equation would correspond to τ_1 and is

$$n\hat{\mu} + n\hat{\tau}_1 = y_{1.}$$

because only the observations in the first treatment contain τ_1 (this gives $y_{1.}$ as the right-hand side), μ and τ_1 appear exactly n times in $y_{1.}$, and all other τ_i appear zero times. In general, the left-hand side of any normal equation is the expected value of the right-hand side.

Now, consider finding the reduction in the sum of squares by fitting a particular model to the data. By fitting a model to the data, we "explain" some of the variability; that is, we reduce the unexplained variability by some amount. The reduction in the unexplained variability is always the sum of the parameter estimates, each multiplied by

the right-hand side of the normal equation that corresponds to that parameter. For example, in a single-factor experiment, the reduction due to fitting the full model $y_{ij} = \mu + \tau_i + \epsilon_{ij}$ is

$$\begin{aligned} R(\mu, \tau) &= \hat{\mu} y_{..} + \hat{\tau}_1 y_{1.} + \hat{\tau}_2 y_{2.} + \cdots + \hat{\tau}_a y_{a.} \\ &= \hat{\mu} y_{..} + \sum_{i=1}^{a} \hat{\tau}_i y_{i.} \end{aligned} \tag{3-55}$$

The notation $R(\mu, \tau)$ means that reduction in the sum of squares from fitting the model containing μ and $\{\tau_i\}$. $R(\mu, \tau)$ is also sometimes called the "regression" sum of squares for the full model $y_{ij} = \mu + \tau_i + \epsilon_{ij}$. The number of degrees of freedom associated with a reduction in the sum of squares, such as $R(\mu, \tau)$, is always equal to the number of linearly independent normal equations. The remaining variability unaccounted for by the model is found from

$$SS_E = \sum_{i=1}^{a} \sum_{j=1}^{n} y_{ij}^2 - R(\mu, \tau) \tag{3-56}$$

This quantity is used in the denominator of the test statistic for $H_0: \tau_1 = \tau_2 = \cdots = \tau_a = 0$.

We now illustrate the general regression significance test for a single-factor experiment and show that it yields the usual one-way analysis of variance. The model is $y_{ij} = \mu + \tau_i + \epsilon_{ij}$, and the normal equations are found from the above rules as

$$\begin{aligned} N\hat{\mu} + n\hat{\tau}_1 + n\hat{\tau}_2 + \cdots + n\hat{\tau}_a &= y_{..} \\ n\hat{\mu} + n\hat{\tau}_1 &= y_{1.} \\ n\hat{\mu} + n\hat{\tau}_2 &= y_{2.} \\ &\vdots \quad\quad \vdots \\ n\hat{\mu} + n\hat{\tau}_a &= y_{a.} \end{aligned}$$

Compare these normal equations with those obtained in Equation 3-52.

Applying the constraint $\sum_{i=1}^{a} \hat{\tau}_i = 0$, the estimators for μ and τ_i are

$$\hat{\mu} = \bar{y}_{..} \qquad \hat{\tau}_i = \bar{y}_{i.} - \bar{y}_{..} \qquad i = 1, 2, \ldots, a$$

The reduction in the sum of squares due to fitting this full model is found from Equation 3-55 as

$$\begin{aligned} R(\mu, \tau) &= \hat{\mu} y_{..} + \sum_{i=1}^{a} \hat{\tau}_i y_{i.} \\ &= (\bar{y}_{..}) y_{..} + \sum_{i=1}^{a} (\bar{y}_{i.} - \bar{y}_{..}) y_{i.} \\ &= \frac{y_{..}^2}{N} + \sum_{i=1}^{a} \bar{y}_{i.} y_{i.} - \bar{y}_{..} \sum_{i=1}^{a} y_{i.} \\ &= \sum_{i=1}^{a} \frac{y_{i.}^2}{n} \end{aligned}$$

which has a degrees of freedom because there are a linearly independent normal equations. The error sum of squares is, from Equation 3-56,

$$SS_E = \sum_{i=1}^{a}\sum_{j=1}^{n} y_{ij}^2 - R(\mu, \tau)$$
$$= \sum_{i=1}^{a}\sum_{j=1}^{n} y_{ij}^2 - \sum_{i=1}^{a} \frac{y_{i.}^2}{n}$$

and has $N - a$ degrees of freedom.

To find the sum of squares resulting from the treatment effects (the $\{\tau_i\}$), we consider the model to be restricted to the null hypothesis; that is, $\tau_i = 0$ for all i. The reduced model is $y_{ij} = \mu + \epsilon_{ij}$. There is only one normal equation for this model:

$$N\hat{\mu} = y_{..}$$

and the estimator of μ is $\hat{\mu} = \bar{y}_{..}$. Thus, the reduction in the sum of squares that results from fitting the reduced model containing only μ is

$$R(\mu) = (\bar{y}_{..})(y_{..}) = \frac{y_{..}^2}{N}$$

Because there is only one normal equation for this reduced model, $R(\mu)$ has one degree of freedom. The sum of squares due to the $\{\tau_i\}$, given that μ is already in the model, is the difference between $R(\mu, \tau)$ and $R(\mu)$, which is

$$R(\tau|\mu) = R(\mu, \tau) - R(\mu)$$
$$= R(\text{Full Model}) - R(\text{Reduced Model})$$
$$= \frac{1}{n}\sum_{i=1}^{a} y_{i.}^2 - \frac{y_{..}^2}{N}$$

with $a - 1$ degrees of freedom, which we recognize from Equation 3-9 as $SS_{\text{Treatments}}$. Making the usual normality assumption, the appropriate statistic for testing $H_0: \tau_1 = \tau_2 = \cdots = \tau_a = 0$ is

$$F_0 = \frac{R(\tau|\mu)/(a-1)}{\left[\sum_{i=1}^{a}\sum_{j=1}^{n} y_{ij}^2 - R(\mu, \tau)\right]/(N-a)}$$

which is distributed as $F_{a-1,N-a}$ under the null hypothesis. This is, of course, the test statistic for the single-factor analysis of variance.

3-10 NONPARAMETRIC METHODS IN THE ANALYSIS OF VARIANCE

3-10.1 The Kruskal–Wallis Test

In situations where the normality assumption is unjustified, the experimenter may wish to use an alternative procedure to the F test analysis of variance that does not depend on

this assumption. Such a procedure has been developed by Kruskal and Wallis (1952). The Kruskal–Wallis test is used to test the null hypothesis that the a treatments are identical against the alternative hypothesis that some of the treatments generate observations that are larger than others. Because the procedure is designed to be sensitive for testing differences in means, it is sometimes convenient to think of the Kruskal–Wallis test as a test for equality of treatment means. The Kruskal–Wallis test is a **nonparametric alternative** to the usual analysis of variance.

To perform a Kruskal–Wallis test, first rank the observations y_{ij} in ascending order and replace each observation by its rank, say R_{ij}, with the smallest observation having rank 1. In the case of ties (observations having the same value), assign the average rank to each of the tied observations. Let $R_{i.}$ be the sum of the ranks in the ith treatment. The test statistic is

$$H = \frac{1}{S^2}\left[\sum_{i=1}^{a}\frac{R_{i.}^2}{n_i} - \frac{N(N+1)^2}{4}\right] \tag{3-57}$$

where n_i is the number of observations in the ith treatment, N is the total number of observations, and

$$S^2 = \frac{1}{N-1}\left[\sum_{i=1}^{a}\sum_{j=1}^{n_i} R_{ij}^2 - \frac{N(N+1)^2}{4}\right] \tag{3-58}$$

Note that S^2 is just the variance of the ranks. If there are no ties, $S^2 = N(N+1)/12$, and the test statistic simplifies to

$$H = \frac{12}{N(N+1)}\sum_{i=1}^{a}\frac{R_{i.}^2}{n_i} - 3(N+1) \tag{3-59}$$

When the number of ties is moderate, there will be little difference between Equations 3-57 and 3-59, and the simpler form (Equation 3-59) may be used. If the n_i are reasonably large, say $n_i \geq 5$, H is distributed approximately as χ^2_{a-1} under the null hypothesis. Therefore, if

$$H > \chi^2_{\alpha,a-1}$$

the null hypothesis is rejected. The P-value approach could also be used.

EXAMPLE 3-12

The data from Example 3-1 and their corresponding ranks are shown in Table 3-14 on the next page. Because there is a fairly large number of ties, we use Equation 3-57 as the test statistic. From Equation 3-58 we find

$$\begin{aligned} S^2 &= \frac{1}{N-1}\left[\sum_{i=1}^{a}\sum_{j=1}^{n_i} R_{ij}^2 - \frac{N(N+1)^2}{4}\right] \\ &= \frac{1}{24}\left[5497.79 - \frac{25(26)^2}{4}\right] \\ &= 53.03 \end{aligned}$$

Table 3-14 Data and Ranks for the Tensile Testing Experiment in Example 3-1

Weight Percentage of Cotton									
15		20		25		30		35	
y_{1j}	R_{1j}	y_{2j}	R_{2j}	y_{3j}	R_{3j}	y_{4j}	R_{4j}	y_{5j}	R_{5j}
7	2.0	12	9.5	14	11.0	19	20.5	7	2.0
7	2.0	17	14.0	18	16.5	25	25.0	10	5.0
15	12.5	12	9.5	18	16.5	22	23.0	11	7.0
11	7.0	18	16.5	19	20.5	19	20.5	15	12.5
9	4.0	18	16.5	19	20.5	23	24.0	11	7.0
$R_{i.}$	27.5		66.0		85.0		113.0		33.5

and the test statistic is

$$H = \frac{1}{S^2}\left[\sum_{i=1}^{a}\frac{R_{i.}^2}{n_i} - \frac{N(N+1)^2}{4}\right]$$

$$= \frac{1}{53.03}\left[5245.0 - \frac{25(26)^2}{4}\right]$$

$$= 19.25$$

Because $H > \chi^2_{0.01,4} = 13.28$, we would reject the null hypothesis and conclude that the treatments differ. (The P-value for $H = 19.25$ is $P = 0.0002$.) This is the same conclusion given by the usual analysis of variance F test.

3-10.2 General Comments on the Rank Transformation

The procedure used in the previous section of replacing the observations by their ranks is called the **rank transformation**. It is a very powerful and widely useful technique. If we were to apply the ordinary F test to the ranks rather than to the original data, we would obtain

$$F_0 = \frac{H/(a-1)}{(N-1-H)/(N-a)} \tag{3-60}$$

as the test statistic [see Conover (1980), p. 337]. Note that, as the Kruskal–Wallis statistic H increases or decreases, F_0 also increases or decreases, so the Kruskal–Wallis test is equivalent to applying the usual analysis of variance to the ranks.

The rank transformation has wide applicability in experimental design problems for which no nonparametric alternative to the analysis of variance exists. This includes many of the designs in subsequent chapters of this book. If the data are ranked and the ordinary F test is applied, an approximate procedure that has good statistical properties results [see Conover and Iman (1976, 1981)]. When we are concerned about the normality assumption or the effect of outliers or "wild" values, we recommend that the usual analysis of variance be performed on both the original data and the ranks. When both procedures give similar results, the analysis of variance assumptions are probably satisfied reasonably well, and the standard analysis is satisfactory. When the two procedures differ, the rank transformation should be preferred because it is less likely to be distorted by nonnormality and unusual observations. In such cases, the experimenter may want to

investigate the use of transformations for nonnormality and examine the data and the experimental procedure to determine if outliers are present and why they have occurred.

3-11 PROBLEMS

3-1. The tensile strength of portland cement is being studied. Four different mixing techniques can be used economically. The following data have been collected:

Mixing Technique	Tensile Strength (lb/in^2)			
1	3129	3000	2865	2890
2	3200	3300	2975	3150
3	2800	2900	2985	3050
4	2600	2700	2600	2765

(a) Test the hypothesis that mixing techniques affect the strength of the cement. Use $\alpha = 0.05$.

(b) Construct a graphical display as described in Section 3-5.3 to compare the mean tensile strengths for the four mixing techniques. What are your conclusions?

(c) Use the Fisher LSD method with $\alpha = 0.05$ to make comparisons between pairs of means.

(d) Construct a normal probability plot of the residuals. What conclusion would you draw about the validity of the normality assumption?

(e) Plot the residuals versus the predicted tensile strength. Comment on the plot.

(f) Prepare a scatter plot of the results to aid the interpretation of the results of this experiment.

3-2. (a) Rework part (b) of Problem 3-1 using Duncan's multiple range test with $\alpha = 0.05$. Does this make any difference in your conclusions?

(b) Rework part (b) of Problem 3-1 using Tukey's test with $\alpha = 0.05$. Do you get the same conclusions from Tukey's test that you did from the graphical procedure and/or Duncan's multiple range test?

(c) Explain the difference between the Tukey and Duncan procedures.

3-3. Reconsider the experiment in Problem 3-1. Find a 95 percent confidence interval on the mean tensile strength of the portland cement produced by each of the four mixing techniques. Also find a 95 percent confidence interval on the difference in means for techniques 1 and 3. Does this aid you in interpreting the results of the experiment?

3-4. An experiment was run to determine whether four specific firing temperatures affect the density of a certain type of brick. The experiment led to the following data:

Temperature	Density				
100	21.8	21.9	21.7	21.6	21.7
125	21.7	21.4	21.5	21.4	
150	21.9	21.8	21.8	21.6	21.5
175	21.9	21.7	21.8	21.4	

(a) Does the firing temperature affect the density of the bricks? Use $\alpha = 0.05$.

(b) Is it appropriate to compare the means using Duncan's multiple range test (for example) in this experiment?

(c) Analyze the residuals from this experiment. Are the analysis of variance assumptions satisfied?

(d) Construct a graphical display of the treatment as described in Section 3-5.3. Does this graph adequately summarize the results of the analysis of variance in part (a)?

3-5. Rework part (d) of Problem 3-4 using the Fisher LSD method. What conclusions can you draw? Explain carefully how you modified the technique to account for unequal sample sizes.

3-6. A manufacturer of television sets is interested in the effect on tube conductivity of four different types of coating for color picture tubes. The following conductivity data are obtained:

Coating Type	Conductivity			
1	143	141	150	146
2	152	149	137	143
3	134	136	132	127
4	129	127	132	129

(a) Is there a difference in conductivity due to coating type? Use $\alpha = 0.05$.
(b) Estimate the overall mean and the treatment effects.
(c) Compute a 95 percent confidence interval estimate of the mean of coating type 4. Compute a 99 percent confidence interval estimate of the mean difference between coating types 1 and 4.
(d) Test all pairs of means using the Fisher LSD method with $\alpha = 0.05$.
(e) Use the graphical method discussed in Section 3-5.3 to compare the means. Which coating type produces the highest conductivity?
(f) Assuming that coating type 4 is currently in use, what are your recommendations to the manufacturer? We wish to minimize conductivity.

3-7. Reconsider the experiment from Problem 3-6. Analyze the residuals and draw conclusions about model adequacy.

3-8. An article in the *ACI Materials Journal* (Vol. 84, 1987, pp. 213–216) describes several experiments investigating the rodding of concrete to remove entrapped air. A 3-inch $\times$ 6-inch cylinder was used, and the number of times this rod was used is the design variable. The resulting compressive strength of the concrete specimen is the response. The data are shown in the following table:

Rodding Level	Compressive Strength		
10	1530	1530	1440
15	1610	1650	1500
20	1560	1730	1530
25	1500	1490	1510

(a) Is there any difference in compressive strength due to the rodding level? Use $\alpha = 0.05$.
(b) Find the P-value for the F statistic in part (a).
(c) Analyze the residuals from this experiment. What conclusions can you draw about the underlying model assumptions?
(d) Construct a graphical display to compare the treatment means as described in Section 3-5.3.

3-9. An article in *Environment International* (Vol. 18, No. 4, 1992) describes an experiment in which the amount of radon released in showers was investigated. Radon-enriched water was used in the experiment, and six different orifice diameters were tested in shower heads. The data from the experiment are shown in the following table:

Orifice Diameter	Radon Released (%)			
0.37	80	83	83	85
0.51	75	75	79	79
0.71	74	73	76	77
1.02	67	72	74	74
1.40	62	62	67	69
1.99	60	61	64	66

(a) Does the size of the orifice affect the mean percentage of radon released? Use $\alpha = 0.05$.
(b) Find the P-value for the F statistic in part (a).
(c) Analyze the residuals from this experiment.
(d) Find a 95 percent confidence interval on the mean percent of radon released when the orifice diameter is 1.40.
(e) Construct a graphical display to compare the treatment means as described in Section 3-5.3 What conclusions can you draw?

3-10. The response time in milliseconds was determined for three different types of circuits that could be used in an automatic valve shutoff mechanism. The results are shown in the following table:

Circuit Type	Response Time				
1	9	12	10	8	15
2	20	21	23	17	30
3	6	5	8	16	7

(a) Test the hypothesis that the three circuit types have the same response time. Use $\alpha = 0.01$.
(b) Use Tukey's test to compare pairs of treatment means. Use $\alpha = 0.01$.
(c) Use the graphical procedure in Section 3-5.3 to compare the treatment means. What conclusions can you draw? How do they compare with the conclusions from part (b)?
(d) Construct a set of orthogonal contrasts, assuming that at the outset of the experiment you suspected the response time of circuit type 2 to be different from the other two.
(e) If you were the design engineer and you wished to minimize the response time, which circuit type would you select?
(f) Analyze the residuals from this experiment. Are the basic analysis of variance assumptions satisfied?

3-11. The effective life of insulating fluids at an accelerated load of 35 kV is being studied. Test data have been obtained for four types of fluids. The results were as follows:

Fluid Type	Life (in h) at 35 kV Load					
1	17.6	18.9	16.3	17.4	20.1	21.6
2	16.9	15.3	18.6	17.1	19.5	20.3
3	21.4	23.6	19.4	18.5	20.5	22.3
4	19.3	21.1	16.9	17.5	18.3	19.8

(a) Is there any indication that the fluids differ? Use $\alpha = 0.05$.
(b) Which fluid would you select, given that the objective is long life?
(c) Analyze the residuals from this experiment. Are the basic analysis of variance assumptions satisfied?

3-12. Four different designs for a digital computer circuit are being studied to compare the amount of noise present. The following data have been obtained:

Circuit Design	Noise Observed				
1	19	20	19	30	8
2	80	61	73	56	80
3	47	26	25	35	50
4	95	46	83	78	97

(a) Is the amount of noise present the same for all four designs? Use $\alpha = 0.05$.
(b) Analyze the residuals from this experiment. Are the analysis of variance assumptions satisfied?
(c) Which circuit design would you select for use? Low noise is best.

3-13. Four chemists are asked to determine the percentage of methyl alcohol in a certain chemical compound. Each chemist makes three determinations, and the results are the following:

Chemist	Percentage of Methyl Alcohol		
1	84.99	84.04	84.38
2	85.15	85.13	84.88
3	84.72	84.48	85.16
4	84.20	84.10	84.55

(a) Do chemists differ significantly? Use $\alpha = 0.05$.
(b) Analyze the residuals from this experiment.
(c) If chemist 2 is a new employee, construct a meaningful set of orthogonal contrasts that might have been useful at the start of the experiment.

3-14. Three brands of batteries are under study. It is suspected that the lives (in weeks) of the three brands are different. Five batteries of each brand are tested with the following results:

Weeks of Life		
Brand 1	Brand 2	Brand 3
100	76	108
96	80	100
92	75	96
96	84	98
92	82	100

(a) Are the lives of these brands of batteries different?
(b) Analyze the residuals from this experiment.
(c) Construct a 95 percent confidence interval estimate on the mean life of battery brand 2. Construct a 99 percent confidence interval estimate on the mean difference between the lives of battery brands 2 and 3.

(d) Which brand would you select for use? If the manufacturer will replace without charge any battery that fails in less than 85 weeks, what percentage would the company expect to replace?

3-15. Four catalysts that may affect the concentration of one component in a three-component liquid mixture are being investigated. The following concentrations are obtained:

Catalyst			
1	2	3	4
58.2	56.3	50.1	52.9
57.2	54.5	54.2	49.9
58.4	57.0	55.4	50.0
55.8	55.3		51.7
54.9			

(a) Do the four catalysts have the same effect on the concentration?
(b) Analyze the residuals from this experiment.
(c) Construct a 99 percent confidence interval estimate of the mean response for catalyst 1.

3-16. An experiment was performed to investigate the effectiveness of five insulating materials. Four samples of each material were tested at an elevated voltage level to accelerate the time to failure. The failure times (in minutes) are shown below:

Material	Failure Time (minutes)			
1	110	157	194	178
2	1	2	4	18
3	880	1256	5276	4355
4	495	7040	5307	10,050
5	7	5	29	2

(a) Do all five materials have the same effect on mean failure time?
(b) Plot the residuals versus the predicted response. Construct a normal probability plot of the residuals. What information is conveyed by these plots?
(c) Based on your answer to part (b) conduct another analysis of the failure time data and draw appropriate conclusions.

3-17. A semiconductor manufacturer has developed three different methods for reducing particle counts on wafers. All three methods are tested on five wafers and the after-treatment particle count obtained. The data are shown below:

Method	Count				
1	31	10	21	4	1
2	62	40	24	30	35
3	53	27	120	97	68

(a) Do all methods have the same effect on mean particle count?
(b) Plot the residuals versus the predicted response. Construct a normal probability plot of the residuals. Are there potential concerns about the validity of the assumptions?
(c) Based on your answer to part (b) conduct another analysis of the particle count data and draw appropriate conclusions.

3-18. Consider testing the equality of the means of two normal populations, where the variances are unknown but are assumed to be equal. The appropriate test procedure is the pooled t test. Show that the pooled t test is equivalent to the single-factor analysis of variance.

3-19. Show that the variance of the linear combination $\sum_{i=1}^{a} c_i y_{i.}$ is $\sigma^2 \sum_{i=1}^{a} n_i c_i^2$.

3-20. In a fixed effects experiment, suppose that there are n observations for each of four treatments. Let Q_1^2, Q_2^2, Q_3^2 be single-degree-of-freedom components for the orthogonal contrasts. Prove that $SS_{\text{Treatments}} = Q_1^2 + Q_2^2 + Q_3^2$.

3-21. Use Bartlett's test to determine if the assumption of equal variances is satisfied in Problem 3-14. Use $\alpha = 0.05$. Did you reach the same conclusion regarding equality of variances by examining residual plots?

3-22. Use the modified Levene test to determine if the assumption of equal variances is satisfied in Problem 3-14. Use $\alpha = 0.05$. Did you reach the same conclusion regarding the equality of variances by examining residual plots?

3-23. Refer to Problem 3-10. If we wish to detect a maximum difference in mean response times of 10 milliseconds with a probability of at least 0.90, what sample size should be used? How would you obtain a preliminary estimate of σ^2?

3-24. Refer to Problem 3-14.

(a) If we wish to detect a maximum difference in battery life of 10 hours with a probability of at least 0.90, what sample size should be used? Discuss how you would obtain a preliminary estimate of σ^2 for answering this question.

(b) If the difference between brands is great enough so that the standard deviation of an observation is increased by 25 percent, what sample size should be used if we wish to detect this with a probability of at least 0.90?

3-25. Consider the experiment in Problem 3-14. If we wish to construct a 95 percent confidence interval on the difference in two mean battery lives that has an accuracy of ± 2 weeks, how many batteries of each brand must be tested?

3-26. Suppose that four normal populations have means of $\mu_1 = 50$, $\mu_2 = 60$, $\mu_3 = 50$, and $\mu_4 = 60$. How many observations should be taken from each population so that the probability of rejecting the null hypothesis of equal population means is at least 0.90? Assume that $\alpha = 0.05$ and that a reasonable estimate of the error variance is $\sigma^2 = 25$.

3-27. Refer to Problem 3-26.

(a) How would your answer change if a reasonable estimate of the experimental error variance were $\sigma^2 = 36$?

(b) How would your answer change if a reasonable estimate of the experimental error variance were $\sigma^2 = 49$?

(c) Can you draw any conclusions about the sensitivity of your answer in this particular situation about how your estimate of σ affects the decision about sample size?

(d) Can you make any recommendations about how we should use this general approach to choosing n in practice?

3-28. Refer to the aluminum smelting experiment described in Section 3-8. Verify that ratio control methods do not affect average cell voltage. Construct a normal probability plot of the residuals. Plot the residuals versus the predicted values. Is there an indication that any underlying assumptions are violated?

3-29. Refer to the aluminum smelting experiment in Section 3-8. Verify the analysis of variance for pot noise summarized in Table 3-13. Examine the usual residual plots and comment on the experimental validity.

3-30. Four different feed rates were investigated in an experiment on a CNC machine producing a component part used in an aircraft auxiliary power unit. The manufacturing engineer in charge of the experiment knows that a critical part dimension of interest may be affected by the feed rate. However, prior experience has indicated that only dispersion effects are likely to be present. That is, changing the feed rate does not affect the *average* dimension, but it could affect dimensional variability. The engineer makes five production runs at

each feed rate and obtains the standard deviation of the critical dimension (in 10^{-3} mm). The data are shown below. Assume that all runs were made in random order.

Feed Rate (in/min)	Production Run				
	1	2	3	4	5
10	0.09	0.10	0.13	0.08	0.07
12	0.06	0.09	0.12	0.07	0.12
14	0.11	0.08	0.08	0.05	0.06
16	0.19	0.13	0.15	0.20	0.11

(a) Does feed rate have any effect on the standard deviation of this critical dimension?
(b) Use the residuals from this experiment to investigate model adequacy. Are there any problems with experimental validity?

3-31. Consider the data shown in Problem 3-10.
(a) Write out the least squares normal equations for this problem, and solve them for $\hat{\mu}$ and $\hat{\tau}_i$, using the usual constraint ($\sum_{i=1}^{3} \hat{\tau}_i = 0$). Estimate $\tau_1 - \tau_2$.
(b) Solve the equations in (a) using the constraint $\hat{\tau}_3 = 0$. Are the estimators $\hat{\tau}_i$ and $\hat{\mu}$ the same as you found in (a)? Why? Now estimate $\tau_1 - \tau_2$ and compare your answer with that for (a). What statement can you make about estimating contrasts in the τ_i?
(c) Estimate $\mu + \tau_1$, $2\tau_1 - \tau_2 - \tau_3$, and $\mu + \tau_1 + \tau_2$ using the two solutions to the normal equations. Compare the results obtained in each case.

3-32. Apply the general regression significance test to the experiment in Example 3-1. Show that the procedure yields the same results as the usual analysis of variance.

3-33. Use the Kruskal–Wallis test for the experiment in Problem 3-11. Compare the conclusions obtained with those from the usual analysis of variance.

3-34. Use the Kruskal–Wallis test for the experiment in Problem 3-12. Are the results comparable to those found by the usual analysis of variance?

3-35. Consider the experiment in Example 3-1. Suppose that the largest observation on tensile strength is incorrectly recorded as 50. What effect does this have on the usual analysis of variance? What effect does it have on the Kruskal–Wallis test?

4 Randomized Blocks, Latin Squares, and Related Designs

4-1 THE RANDOMIZED COMPLETE BLOCK DESIGN

In any experiment, variability arising from a nuisance factor can affect the results. Generally, we define a **nuisance factor** as a design factor that probably has an effect on the response, but we are not interested in that effect. Sometimes a nuisance factor is **unknown and uncontrolled**; that is, we don't know that the factor exists and it may even be changing levels while we are conducting the experiment. **Randomization** is the design technique used to guard against such a "lurking" nuisance factor. In other cases, the nuisance factor is **known but uncontrollable**. If we can at least observe the value that the nuisance factor takes on at each run of the experiment, we can compensate for it in the statistical analysis by using the **analysis of covariance**, a technique we will discuss in Chapter 14. When the nuisance source of variability is **known and controllable**, a design technique called **blocking** can be used to systematically eliminate its effect on the statistical comparisons among treatments. Blocking is an extremely important design technique, used extensively in industrial experimentation, and is the subject of this chapter.

To illustrate the general idea, suppose we wish to determine whether or not four different tips produce different readings on a hardness testing machine. An experiment such as this might be part of a gauge capability study. The machine operates by pressing the tip into a metal test coupon, and from the depth of the resulting depression, the hardness of the coupon can be determined. The experimenter has decided to obtain four observations for each tip. There is only one factor—tip type—and a completely randomized single-factor design would consist of randomly assigning each one of the $4 \times 4 = 16$ runs to an **experimental unit**, that is, a metal coupon, and observing the hardness reading that results. Thus, 16 different metal test coupons would be required in this experiment, one for each run in the design.

There is a potentially serious problem with a completely randomized experiment in this design situation. If the metal coupons differ slightly in their hardness, as might

Table 4-1 Randomized Complete Block Design for the Hardness Testing Experiment

	Test Coupon			
Type of Tip	1	2	3	4
1	9.3	9.4	9.6	10.0
2	9.4	9.3	9.8	9.9
3	9.2	9.4	9.5	9.7
4	9.7	9.6	10.0	10.2

happen if they are taken from ingots that are produced in different heats, the experimental units (the coupons) will contribute to the variability observed in the hardness data. As a result, the experimental error will reflect *both* random error *and* variability between coupons.

We would like to make the experimental error as small as possible; that is, we would like to remove the variability between coupons from the experimental error. A design that would accomplish this requires the experimenter to test each tip once on each of four coupons. This design, shown in Table 4-1, is called a **randomized complete block design (RCBD)**. The observed response is the Rockwell C scale hardness minus 40. The word "complete" indicates that each block (coupon) contains all the treatments (tips). By using this design, the blocks, or coupons, form a more homogeneous experimental unit on which to compare the tips. Effectively, this design strategy improves the accuracy of the comparisons among tips by eliminating the variability among the coupons. Within a block, the order in which the four tips are tested is randomly determined. Notice the similarity of this design problem to the one of Section 2-5 in which the paired t-test was discussed. The randomized complete block design is a generalization of that concept.

The RCBD is one of the most widely used experimental designs. Situations for which the RCBD is appropriate are numerous. Units of test equipment or machinery are often different in their operating characteristics and would be a typical blocking factor. Batches of raw material, people, and time are also common nuisance sources of variability in an experiment that can be systematically controlled through blocking.

Blocking may also be useful in situations that do not necessarily involve nuisance factors. For example, suppose that a chemical engineer is interested in the effect of catalyst feed rate on the viscosity of a polymer. She knows that there are several factors, such as raw material source, temperature, operator, and raw material purity that are very difficult to control in the full-scale process. Therefore she decides to test the catalyst feed rate factor in blocks, where each block consists of some combination of these uncontrollable factors. In effect, she is using the blocks to test the **robustness** of her process variable (feed rate) to conditions she cannot easily control. For more discussion of this, see Coleman and Montgomery (1993).

4-1.1 Statistical Analysis of the RCBD

Suppose we have, in general, a treatments that are to be compared and b blocks. The randomized complete block design is shown in Figure 4-1 on the next page. There is one observation per treatment in each block, and the order in which the treatments are run

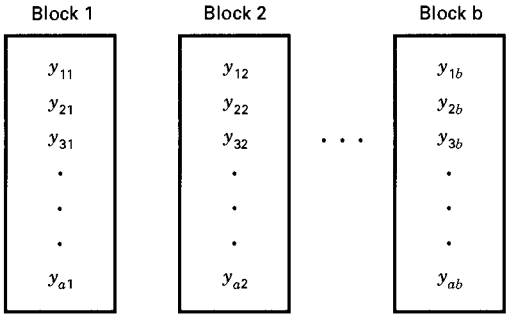


Figure 4-1 The randomized complete block design.

within each block is determined randomly. Because the only randomization of treatments is within the blocks, we often say that the blocks represent a **restriction on randomization.**

The **statistical model** for the RCBD can be written in several ways. The traditional model is an **effects model**:

$$y_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij} \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \end{cases} \tag{4-1}$$

where μ is an overall mean, τ_i is the effect of the ith treatment, β_j is the effect of the jth block, and ϵ_{ij} is the usual NID $(0, \sigma^2)$ random error term. We will initially consider treatments and blocks to be fixed factors. Just as in the single-factor experimental design model in Chapter 3, the effects model for the RCBD is an overspecified model. Consequently, we usually think of the treatment and block effects as deviations from the overall mean so that

$$\sum_{i=1}^{a} \tau_i = 0 \qquad \text{and} \qquad \sum_{j=1}^{b} \beta_j = 0$$

It is also possible to use a **means model** for the RCBD, say

$$y_{ij} = \mu_{ij} + \epsilon_{ij} \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \end{cases}$$

where $\mu_{ij} = \mu + \tau_i + \beta_j$. However, we will use the effects model in Equation 4-1 throughout this chapter.

In an experiment involving the RCBD, we are interested in testing the equality of the treatment means. Thus, the hypotheses of interest are

$$H_0: \mu_1 = \mu_2 = \cdots = \mu_a$$
$$H_1: \text{at least one } \mu_i \neq \mu_j$$

Because the ith treatment mean $\mu_i = (1/b)\sum_{j=1}^{b}(\mu + \tau_i + \beta_j) = \mu + \tau_i$, an equivalent way to write the above hypotheses is in terms of the treatment effects, say

$$H_0: \tau_1 = \tau_2 = \cdots = \tau_a = 0$$
$$H_1: \tau_i \neq 0 \text{ at least one } i$$

Let $y_{i.}$ be the total of all observations taken under treatment i, $y_{.j}$ be the total of all observations in block j, $y_{..}$ be the grand total of all observations, and $N = ab$ be the total number of observations. Expressed mathematically,

$$y_{i.} = \sum_{j=1}^{b} y_{ij} \qquad i = 1, 2, \ldots, a \tag{4-2}$$

$$y_{.j} = \sum_{i=1}^{a} y_{ij} \qquad j = 1, 2, \ldots, b \tag{4-3}$$

and

$$y_{..} = \sum_{i=1}^{a} \sum_{j=1}^{b} y_{ij} = \sum_{i=1}^{a} y_{i.} = \sum_{j=1}^{b} y_{.j} \tag{4-4}$$

Similarly, $\bar{y}_{i.}$ is the average of the observations taken under treatment i, $\bar{y}_{.j}$ is the average of the observations in block j, and $\bar{y}_{..}$ is the grand average of all observations. That is,

$$\bar{y}_{i.} = y_{i.}/b \qquad \bar{y}_{.j} = y_{.j}/a \qquad \bar{y}_{..}/N \tag{4-5}$$

We may express the total corrected sum of squares as

$$\sum_{i=1}^{a} \sum_{j=1}^{b} (y_{ij} - \bar{y}_{..})^2 = \sum_{i=1}^{a} \sum_{j=1}^{b} [(\bar{y}_{i.} - \bar{y}_{..}) + (\bar{y}_{.j} - \bar{y}_{..}) + (y_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..})]^2 \tag{4-6}$$

By expanding the right-hand side of Equation 4-6, we obtain

$$\begin{aligned}\sum_{i=1}^{a} \sum_{j=1}^{b} (y_{ij} - \bar{y}_{..})^2 = {} & b \sum_{i=1}^{a} (\bar{y}_{i.} - \bar{y}_{..})^2 + a \sum_{j=1}^{b} (\bar{y}_{.j} - \bar{y}_{..})^2 \\ & + \sum_{i=1}^{a} \sum_{j=1}^{b} (y_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..})^2 + 2 \sum_{i=1}^{a} \sum_{j=1}^{b} (\bar{y}_{i.} - \bar{y}_{..})(\bar{y}_{.j} - \bar{y}_{..}) \\ & + 2 \sum_{i=1}^{a} \sum_{j=1}^{b} (\bar{y}_{.j} - \bar{y}_{..})(y_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..}) \\ & + 2 \sum_{i=1}^{a} \sum_{j=1}^{b} (\bar{y}_{i.} - \bar{y}_{..})(y_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..})\end{aligned}$$

Simple but tedious algebra proves that the three cross-products are zero. Therefore,

$$\begin{aligned}\sum_{i=1}^{a} \sum_{j=1}^{b} (y_{ij} - \bar{y}_{..})^2 = {} & b \sum_{i=1}^{a} (\bar{y}_{i.} - \bar{y}_{..})^2 + a \sum_{j=1}^{b} (\bar{y}_{.j} - \bar{y}_{..})^2 \\ & + \sum_{i=1}^{a} \sum_{j=1}^{b} (y_{ij} - \bar{y}_{.j} - \bar{y}_{i.} + \bar{y}_{..})^2\end{aligned} \tag{4-7}$$

represents a partition of the total sum of squares. Expressing the sums of squares in Equation 4-7 symbolically, we have

$$SS_T = SS_{\text{Treatments}} + SS_{\text{Blocks}} + SS_E \tag{4-8}$$

Because there are N observations, SS_T has $N - 1$ degrees of freedom. There are a treatments and b blocks, so $SS_{\text{Treatments}}$ and SS_{Blocks} have $a - 1$ and $b - 1$ degrees of freedom, respectively. The error sum of squares is just a sum of squares between

cells minus the sum of squares for treatments and blocks. There are ab cells with $ab - 1$ degrees of freedom between them, so SS_E has $ab - 1 - (a - 1) - (b - 1) = (a - 1)(b - 1)$ degrees of freedom. Furthermore, the degrees of freedom on the right-hand side of Equation 4-8 add to the total on the left; therefore, making the usual normality assumptions on the errors, one may use Theorem 3-1 to show that $SS_{\text{Treatments}}/\sigma^2$, $SS_{\text{Blocks}}/\sigma^2$, and SS_E/σ^2 are independently distributed chi-square random variables. Each sum of squares divided by its degrees of freedom is a mean square. The expected value of the mean squares, if treatments and blocks are fixed, can be shown to be

$$E(MS_{\text{Treatments}}) = \sigma^2 + \frac{b\sum_{i=1}^{a}\tau_i^2}{a-1}$$

$$E(MS_{\text{Blocks}}) = \sigma^2 + \frac{a\sum_{j=1}^{b}\beta_j^2}{b-1}$$

$$E(MS_E) = \sigma^2$$

Therefore, to test the equality of treatment means, we would use the test statistic

$$F_0 = \frac{MS_{\text{Treatments}}}{MS_E}$$

which is distributed as $F_{a-1,(a-1)(b-1)}$ if the null hypothesis is true. The critical region is the upper tail of the F distribution, and we would reject H_0 if $F_0 > F_{\alpha,a-1,(a-1)(b-1)}$.

We may also be interested in comparing block means because, if these means do not differ greatly, blocking may not be necessary in future experiments. From the expected mean squares, it seems that the hypothesis $H_0: \beta_j = 0$ may be tested by comparing the statistic $F_0 = MS_{\text{Blocks}}/MS_E$ to $F_{\alpha,b-1,(a-1)(b-1)}$. However, recall that randomization has been applied only to treatments *within* blocks; that is, the blocks represent a **restriction on randomization**. What effect does this have on the statistic $F_0 = MS_{\text{Blocks}}/MS_E$? Some differences in treatment of this question exists. For example, Box, Hunter, and Hunter (1978) point out that the usual analysis of variance F test can be justified on the basis of randomization only,[1] without direct use of the normality assumption. They further observe that the test to compare block means cannot appeal to such a justification because of the randomization restriction; but if the errors are NID(0, σ^2), the statistic $F_0 = MS_{\text{Blocks}}/MS_E$ can be used to compare block means. On the other hand, Anderson and McLean (1974) argue that the randomization restriction prevents this statistic from being a meaningful test for comparing block means and that this F ratio really is a test for the equality of the block means plus the randomization restriction [which they call a restriction error; see Anderson and McLean (1974) for further details].

In practice, then, what do we do? Because the normality assumption is often questionable, to view $F_0 = MS_{\text{Blocks}}/MS_E$ as an exact F test on the equality of block means is not a good general practice. For that reason, we exclude this F test from the analysis of variance table. However, as an approximate procedure to investigate the effect of the blocking variable, examining the ratio of MS_{Blocks} to MS_E is certainly reasonable. If this

[1] Actually, the normal-theory F distribution is an approximation to the randomization distribution generated by calculating F_0 from every possible assignment of the responses to the treatments.

Table 4-2 Analysis of Variance for a Randomized Complete Block Design

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Treatments	$SS_{\text{Treatments}}$	$a - 1$	$\frac{SS_{\text{Treatments}}}{a - 1}$	$\frac{MS_{\text{Treatments}}}{MS_E}$
Blocks	SS_{Blocks}	$b - 1$	$\frac{SS_{\text{Blocks}}}{b - 1}$	
Error	SS_E	$(a - 1)(b - 1)$	$\frac{SS_E}{(a - 1)(b - 1)}$	
Total	SS_T	$N - 1$		

ratio is large, it implies that the blocking factor has a large effect and that the noise reduction obtained by blocking was probably helpful in improving the precision of the comparison of treatment means.

The procedure is usually summarized in an analysis of variance table, such as the one shown in Table 4-2. The computing would usually be done with a statistical software package. However, manual computing formulas for the sums of squares may be obtained for the elements in Equation 4-7 by expressing them in terms of treatment and block totals. These computing formulas are

$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij}^2 - \frac{y_{..}^2}{N} \tag{4-9}$$

$$SS_{\text{Treatments}} = \frac{1}{b}\sum_{i=1}^{a} y_{i.}^2 - \frac{y_{..}^2}{N} \tag{4-10}$$

$$SS_{\text{Blocks}} = \frac{1}{a}\sum_{j=1}^{b} y_{.j}^2 - \frac{y_{..}^2}{N} \tag{4-11}$$

and the error sum of squares is obtained by subtraction as

$$SS_E = SS_T - SS_{\text{Treatments}} - SS_{\text{Blocks}} \tag{4-12}$$

EXAMPLE 4-1

Consider the hardness testing experiment described in Section 4-1. There are four tips and four available metal coupons. Each tip is tested once on each coupon, resulting in a randomized complete block design. The data obtained are repeated for convenience in Table 4-3. Remember that the *order* in which the tips were tested on a particular coupon was determined randomly. To simplify the calculations, we code the original data by

Table 4-3 Randomized Complete Block Design for the Hardness Testing Experiment

	Coupon (Block)			
Type of Tip	1	2	3	4
1	9.3	9.4	9.6	10.0
2	9.4	9.3	9.8	9.9
3	9.2	9.4	9.5	9.7
4	9.7	9.6	10.0	10.2

Table 4-4 Coded Data for the Hardness Testing Experiment

	Coupon (Block)				
Type of Tip	1	2	3	4	$y_{i.}$
1	−2	−1	1	5	3
2	−1	−2	3	4	4
3	−3	−1	0	2	−2
4	2	1	5	7	15
$y_{.j}$	−4	−3	9	18	$20 = y_{..}$

subtracting 9.5 from each observation and multiplying the result by 10. This yields the data in Table 4-4. The sums of squares are obtained as follows:

$$SS_T = \sum_{i=1}^{4}\sum_{j=1}^{4} y_{ij}^2 - \frac{y_{..}^2}{N}$$

$$= 154.00 - \frac{(20)^2}{16} = 129.00$$

$$SS_{\text{Treatments}} = \frac{1}{b}\sum_{i=1}^{4} y_{i.}^2 - \frac{y_{..}^2}{N}$$

$$= \frac{1}{4}[(3)^2 + (4)^2 + (-2)^2 + (15)^2] - \frac{(20)^2}{16} = 38.50$$

$$SS_{\text{Blocks}} = \frac{1}{a}\sum_{j=1}^{4} y_{.j}^2 - \frac{y_{..}^2}{N}$$

$$= \frac{1}{4}[(-4)^2 + (-3)^2 + (9)^2 + (18)^2] - \frac{(20)^2}{16} = 82.50$$

$$SS_E = SS_T - SS_{\text{Treatments}} - SS_{\text{Blocks}}$$

$$= 129.00 - 38.50 - 82.50 = 8.00$$

The analysis of variance is shown in Table 4-5. Using $\alpha = 0.05$, the critical value of F is $F_{0.05,3,9} = 3.86$. Because $14.44 > 3.86$, we conclude that the type of tip affects the mean hardness reading. The P-value for the test is also quite small. Also, the coupons (blocks) seem to differ significantly, because the mean square for blocks is large relative to error.

It is interesting to observe the results we would have obtained had we not been aware of randomized block designs. Suppose we used four coupons, randomly assigned the tips to each, and (by chance) the same design resulted as in Table 4-3. The incorrect analysis of these data as a completely randomized single-factor design is shown in Table 4-6.

Table 4-5 Analysis of Variance for the Hardness Testing Experiment

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Treatments (type of tip)	38.50	3	12.83	14.44	0.0009
Blocks (coupons)	82.50	3	27.50		
Error	8.00	9	0.89		
Total	129.00	15			

Table 4-6 Incorrect Analysis of the Hardness Testing Experiment as a Completely Randomized Design

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Type of tip	38.50	3	12.83	1.70
Error	90.50	12	7.54	
Total	129.00	15		

Because $F_{0.05,3,12} = 3.49$, the hypothesis of equal mean hardness measurements from the four tips cannot be rejected. Thus, the randomized block design reduces the amount of noise in the data sufficiently for differences among the four tips to be detected. This illustrates a very important point. If an experimenter fails to block when he or she should have, the effect may be to inflate the experimental error so much that important differences among the treatment means may be undetectable.

Sample Computer Output

Condensed computer output for the hardness testing data in Example 4-1, obtained from Design-Expert, is shown in Figure 4-2 on page 134. Recall that the original analysis in Table 4-5 used *coded* data. (The raw responses were coded by subtracting 9.5 and multiplying the result by 10.) The computer analysis used the raw responses. Consequently, the sums of squares in Figure 4-2 are equal to those in Table 4-5 divided by 100 (note that Design-Expert has rounded the sums of squares to two decimal places).

The residuals are listed at the bottom of the computer output. They are calculated as

$$e_{ij} = y_{ij} - \hat{y}_{ij}$$

and, as we will later show, the fitted values are $\hat{y}_{ij} = \bar{y}_{i.} + \bar{y}_{.j} - \bar{y}_{..}$, so

$$e_{ij} = y_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..} \tag{4-13}$$

In the next section, we will show how the residuals are used in **model adequacy checking**.

Multiple Comparisons

If the treatments in an RCBD are fixed, and the analysis indicates a significant difference in treatment means, the experimenter is usually interested in multiple comparisons to discover *which* treatment means differ. Any of the multiple comparison procedures discussed in Chapter 3 (Section 3-5) may be used for this purpose. In the formulas of Section 3-5, simply replace the number of replicates in the single-factor completely randomized design (n) by the number of blocks (b). Also, remember to use the number of error degrees of freedom for the randomized block $[(a - 1)(b - 1)]$ instead of those for the completely randomized design $[a(n - 1)]$.

The Design-Expert output in Figure 4-2 illustrates the Fisher LSD procedure. Notice that if we use $\alpha = 0.05$, we would conclude that $\mu_2 = \mu_3$. Now because $\bar{y}_{3.} \leqslant \bar{y}_{1.} \leqslant \bar{y}_{2.}$ (that is, the means $\bar{y}_{2.}$ and $\bar{y}_{3.}$ span some of the remaining means), we can immediately conclude that $\mu_1 = \mu_2 = \mu_3$. Furthermore, μ_4 is different from all three other means. Thus we conclude that tip type 4 produces a mean hardness that is significantly higher than the mean hardness readings from the other three types of tips.

We can also use the graphical procedure of Chapter 3 (Section 3-5.1) to compare tip

Response: Hardness in Rockwell C
ANOVA for Selected Factorial Model
Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Block	0.82	3	0.27			
Model	0.38	3	0.13	14.44	0.0009	significant
A	*0.38*	*3*	*0.13*	*14.44*	*0.0009*	
Residual	0.080	9	8.889E-003			
Cor Total	1.29	15				

Std. Dev.	0.094	R-Squared	0.8280
Mean	9.63	Adj R-Squared	0.7706
C.V.	0.98	Pred R-Squared	0.4563
PRESS	0.25	Adeq Precision	15.635

Treatment Means (Adjusted, If Necessary)

	Estimated Mean	Standard Error
1-A1	9.57	0.47
2-A2	9.60	0.47
3-A3	9.45	0.47
4-A4	9.88	0.47

Treatment	Mean Difference	DF	Standard Error	t for H_0 Coeff=0	Prob > |t|
1 vs 2	−0.025	1	0.067	−0.38	0.7163
1 vs 3	0.13	1	0.067	1.87	0.0935
1 vs 4	−0.30	1	0.067	−4.50	0.0015
2 vs 3	0.15	1	0.067	2.25	0.0510
2 vs 4	−0.27	1	0.067	−4.12	0.0026
3 vs 4	−0.43	1	0.067	−6.37	0.0001

Diagnostics Case Statistics

Standard Order	Actual Value	Predicted Value	Residual	Leverage	Student Residual	Cook's Distance	Outlier t
1	9.30	9.35	−0.050	0.438	−0.707	0.056	−0.686
2	9.40	9.38	0.025	0.438	0.354	0.014	0.336
3	9.60	9.67	−0.075	0.437	−1.061	0.125	−1.069
4	10.00	9.90	0.100	0.438	1.414	0.222	1.512
5	9.40	9.38	0.025	0.438	0.354	0.014	0.336
6	9.30	9.40	−0.100	0.437	−1.414	0.222	−1.512
7	9.80	9.70	0.100	0.437	1.414	0.222	1.512
8	9.90	9.93	−0.025	0.437	−0.354	0.014	−0.336
9	9.20	9.22	−0.025	0.438	−0.354	0.014	−0.336
10	9.40	9.25	0.150	0.437	2.121	0.500	2.828
11	9.50	9.55	−0.050	0.437	−0.707	0.056	−0.686
12	9.70	9.78	−0.075	0.437	−1.061	0.125	−1.069
13	9.70	9.65	0.050	0.438	0.707	0.056	0.686
14	9.60	9.68	−0.075	0.437	−1.061	0.125	−1.069
15	10.00	9.97	0.025	0.437	0.354	0.014	0.336
16	10.20	10.20	0.000	0.437	0.000	0.000	0.000

Figure 4-2 Design-Expert output (condensed) for Example 4-1.

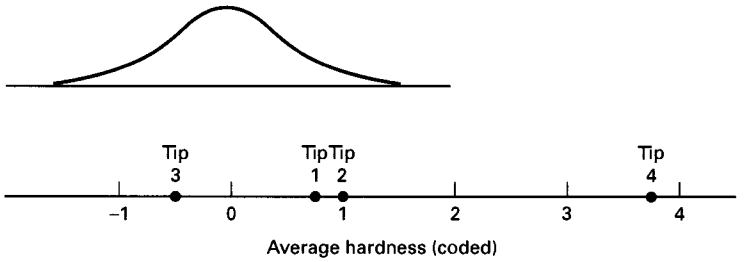


Figure 4-3 Tip type means relative to a scaled t distribution with a scale factor $\sqrt{MS_E/b} = \sqrt{0.89/4} = 0.47$.

type means. Figure 4-3 plots the four tip type means from Example 4-1 relative to a scaled t distribution with a scale factor $\sqrt{MS_E/b} = \sqrt{0.89/4} = 0.47$. This plot indicates that tips 1, 2, and 3 probably produce identical average hardness measurements but that tip 4 produces a much higher mean hardness. This figure confirms the results from the Fisher LSD test in the Design-Expert output in Figure 4-2.

4-1.2 Model Adequacy Checking

We have previously discussed the importance of checking the adequacy of the assumed model. Generally, we should be alert for potential problems with the normality assumption, unequal error variance by treatment or block, and block–treatment interaction. As in the completely randomized design, residual analysis is the major tool used in this diagnostic checking. The residuals for the randomized block design in Example 4-1 are listed at the bottom of the Design-Expert output in Figure 4-2. The coded residuals would be found by multiplying these residuals by 10. The observations, fitted values, and residuals for the coded hardness testing data in Example 4-1 are as follows:

y_{ij}	$\hat{y}_{ij}$	e_{ij}
−2.00	−1.50	−0.50
−1.00	−1.25	0.25
1.00	1.75	−0.75
5.00	4.00	1.00
−1.00	−1.25	0.25
−2.00	−1.00	−1.00
3.00	2.00	1.00
4.00	4.25	−0.25
−3.00	−2.75	−0.25
−1.00	−2.50	1.50
0.00	0.50	−0.50
2.00	2.75	−0.75
2.00	1.50	0.50
1.00	1.75	−0.75
5.00	4.75	0.25
7.00	7.00	0.00

A normal probability plot and a dot diagram of these residuals are shown in Figure 4-4 on page 136. There is no severe indication of nonnormality, nor is there any evidence pointing to possible outliers. Figure 4-5 (page 137) shows plots of the residuals by type

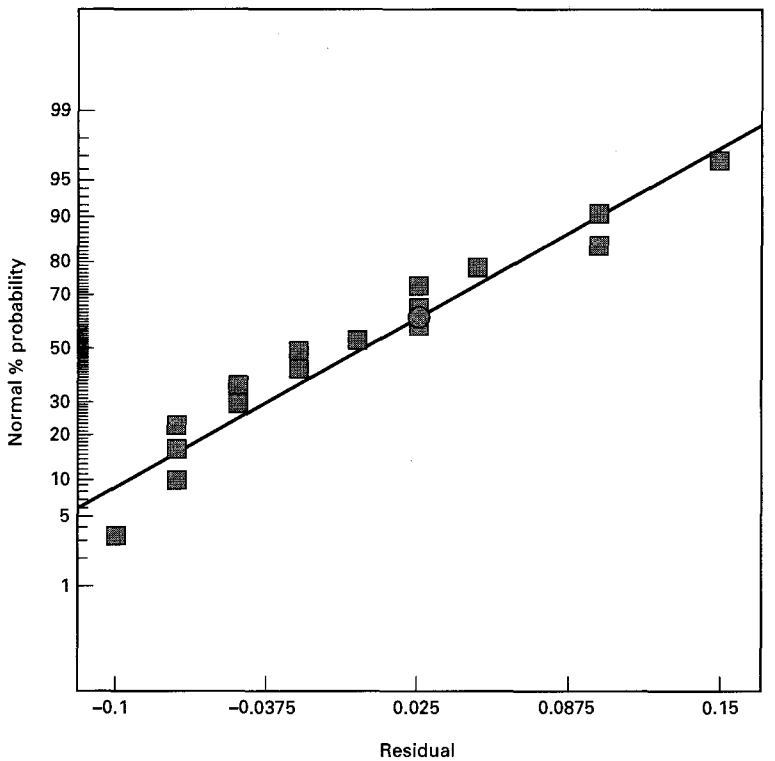


Figure 4-4 Normal probability plot of residuals for Example 4-1.

of tip or treatment and by coupon or block. These plots could be, potentially, very informative. If there is more scatter in the residuals for a particular tip, that could indicate that this tip produces more erratic hardness readings than the others. More scatter in the residuals for a particular test coupon could indicate that the coupon is not of uniform hardness. However, in our example, Figure 4-5 gives no indication of inequality of variance by treatment or by block. Figure 4-6 (on the facing page) plots the residuals versus the fitted values $\hat{y}_{ij}$. There should be no relationship between the size of the residuals and the fitted values $\hat{y}_{ij}$. This plot reveals nothing of unusual interest.

Sometimes the plot of residuals versus $\hat{y}_{ij}$ has a curvilinear shape; for example, there may be a tendency for negative residuals to occur with low $\hat{y}_{ij}$ values, positive residuals with intermediate $\hat{y}_{ij}$ values, and negative residuals with high $\hat{y}_{ij}$ values. This type of pattern is suggestive of **interaction** between blocks and treatments. If this pattern occurs, a transformation should be used in an effort to eliminate or minimize the interaction. In Chapter 5 (Section 5-3.7), we describe a statistical test that can be used to detect the presence of interaction in a randomized block design.

4-1.3 Some Other Aspects of the Randomized Complete Block Design

Additivity of the Randomized Block Model

The linear statistical model that we have used for the randomized block design

$$y_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij}$$

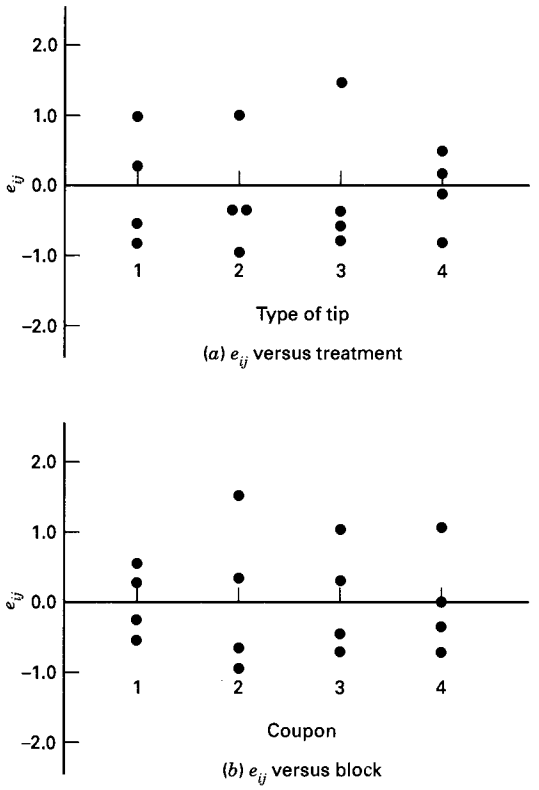


Figure 4-5 Plot of residuals by tip type (treatment) and by coupon (block) for Example 4-1.

is completely **additive**. This says that, for example, if the first treatment causes the expected response to increase by five units ($\tau_1 = 5$) and if the first block increases the expected response by 2 units ($\beta_1 = 2$), the expected increase in response of *both* treatment 1 *and* block 1 together is $E(y_{11}) = \mu + \tau_1 + \beta_1 = \mu + 5 + 2 = \mu + 7$. In general,

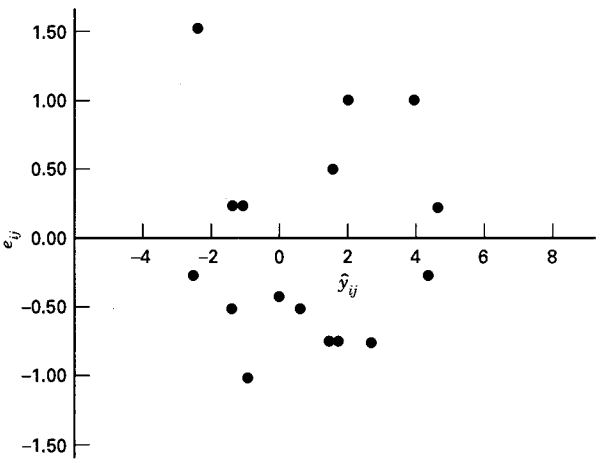


Figure 4-6 Plot of residuals versus $\hat{y}_{ij}$ for Example 4-1.

treatment 1 *always* increases the expected response by 5 units over the sum of the overall mean and the block effect.

Although this simple additive model is often useful, there are situations where it is inadequate. Suppose, for example, that we are comparing four formulations of a chemical product using six batches of raw material; the raw material batches are considered blocks. If an impurity in batch 2 affects formulation 2 adversely, resulting in an unusually low yield, but does not affect the other formulations, an **interaction** between formulations (or treatments) and batches (or blocks) has occurred. Similarly, interactions between treatments and blocks can occur when the response is measured on the wrong scale. Thus, a relationship that is multiplicative in the original units, say

$$E(y_{ij}) = \mu\tau_i\beta_j$$

is linear or additive in a log scale since, for example,

$$\ln E(y_{ij}) = \ln \mu + \ln \tau_i + \ln \beta_j$$

or

$$E(y_{ij}^*) = \mu^* + \tau_i^* + \beta_j^*$$

Although this type of interaction can be eliminated by a transformation, not all interactions are so easily treated. For example, transformations do not eliminate the formulation–batch interaction discussed previously. Residual analysis and other diagnostic checking procedures can be helpful in detecting nonadditivity.

If interaction is present, it can seriously affect and possibly invalidate the analysis of variance. In general, the presence of interaction inflates the error mean square and may adversely affect the comparison of treatment means. In situations where both factors, as well as their possible interaction, are of interest, **factorial designs** must be used. These designs are discussed extensively in Chapters 5 through 9.

Random Treatments and Blocks

Although we have described the test procedure considering treatments and blocks as fixed factors, the same analysis procedure is used if either the treatments or blocks (or both) are random. However, there are some changes in the interpretation of the results. For example, if the blocks are random, which is quite often the case, we expect the comparisons among the treatments to be the same throughout the **population of blocks** from which those used in the experiment were randomly selected. There are also corresponding changes in the expected mean squares. For example, if the blocks are independent random variables with common variance, $E(MS_{\text{Blocks}}) = \sigma^2 + a\sigma_\beta^2$, where σ_β^2 is the variance component of the block effects. In any event, $E(MS_{\text{Treatments}})$ is always free of any block effect, and the test statistic for between-treatment variability is always $F_0 = MS_{\text{Treatments}}/MS_E$.

In situations where the blocks are random, if treatment–block interaction is present, the test on treatment means is unaffected by the interaction. The reason for this is that the expected mean squares for treatments and error *both* contain the interaction effect; consequently, the test for differences in treatment means may be conducted as usual by comparing the treatment mean square to the error mean square. This procedure does not yield any information on the interaction.

Choice of Sample Size

Choosing the **sample size**, or the **number of blocks** to run, is an important decision when using an RCBD. Increasing the number of blocks increases the number of replicates and the number of error degrees of freedom, making the design more sensitive. Any of the techniques discussed in Chapter 3 (Section 3-7) for selecting the number of replicates to run in a completely randomized single-factor experiment may be applied directly to the RCBD. For the case of a fixed factor, the operating characteristic curves in Appendix Chart V may be used with

$$\Phi^2 = \frac{b\sum_{i=1}^{a}\tau_i^2}{a\sigma^2} \tag{4-14}$$

where there are $a - 1$ numerator degrees of freedom and $(a - 1)(b - 1)$ denominator degrees of freedom.

EXAMPLE 4-2

Consider the hardness testing problem described in Example 4-1. Suppose that we wish to determine the appropriate number of blocks to run if we are interested in detecting a true maximum difference in mean hardness readings of 0.4 with a high probability and a reasonable estimate of the standard deviation of the errors is $\sigma = 0.1$. (These values are given in the *original* units; recall that the analysis of variance was performed using *coded* data.) From Equation 3-49, the minimum value of Φ^2 is (writing b, the number of blocks, for n)

$$\Phi^2 = \frac{bD^2}{2a\sigma^2}$$

where D is the maximum difference we wish to detect. Thus,

$$\Phi^2 = \frac{b(0.4)^2}{2(4)(0.1)^2} = 2.0b$$

If we use $b = 3$ blocks, $\Phi = \sqrt{2.0b} = \sqrt{2.0(3)} = 2.45$, and there are $(a - 1)(b - 1) = 3(2) = 6$ error degrees of freedom. Appendix Chart V with $\nu_1 = a - 1 = 3$ and $\alpha = 0.05$ indicates that the β risk for this design is approximately 0.10 (power $= 1 - \beta = 0.90$). If we use $b = 4$ blocks, $\Phi = \sqrt{2.0b} = \sqrt{2.0(4)} = 2.83$, with $(a - 1)(b - 1) = 3(3) = 9$ error degrees of freedom, and the corresponding β risk is approximately 0.03 (power $= 1 - \beta = 0.97$). Either three or four blocks will result in a design having a high probability of detecting the difference between the mean hardness readings considered important. Because coupons (blocks) are inexpensive and readily available and the cost of testing is low, the experimenter decides to use four blocks.

Estimating Missing Values

When using the RCBD, sometimes an observation in one of the blocks is missing. This may happen because of carelessness or error or for reasons beyond our control, such as unavoidable damage to an experimental unit. A missing observation introduces a new problem into the analysis because treatments are no longer **orthogonal to blocks**; that

Table 4-7 Randomized Complete Block Design for the Hardness Testing Experiment with One Missing Value

	Coupon (Block)			
Type of Tip	1	2	3	4
1	−2	−1	1	5
2	−1	−2	x	4
3	−3	−1	0	2
4	2	1	5	7

is, every treatment does not occur in every block. There are two general approaches to the missing value problem. The first is an **approximate analysis** in which the missing observation is estimated and the usual analysis of variance is performed just as if the estimated observation were real data, with the error degrees of freedom reduced by 1. This approximate analysis is the subject of this section. The second is an **exact analysis**, which is discussed in Section 4-1.4.

Suppose the observation y_{ij} for treatment i in block j is missing. Denote the missing observation by x. As an illustration, suppose that in the hardness testing experiment of Example 4-1 coupon 3 was broken while tip 2 was being tested and that data point could not be obtained. The data might appear as in Table 4-7.

In general, we will let $y'_{..}$ represent the grand total with one missing observation, $y'_{i.}$ represent the total for the treatment with one missing observation, and $y'_{.j}$ be the total for the block with one missing observation. Suppose we wish to estimate the missing observation x so that x will have a minimum contribution to the error sum of squares. Because $SS_E = \Sigma_{i=1}^{a}\Sigma_{j=1}^{b}(y_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..})^2$, this is equivalent to choosing x to minimize

$$SS_E = \sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij}^2 - \frac{1}{b}\sum_{i=1}^{a}\left(\sum_{j=1}^{b} y_{ij}\right)^2 - \frac{1}{a}\sum_{j=1}^{b}\left(\sum_{i=1}^{a} y_{ij}\right)^2 + \frac{1}{ab}\left(\sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij}\right)^2$$

or

$$SS_E = x^2 - \frac{1}{b}(y'_{i.} + x)^2 - \frac{1}{a}(y'_{.j} + x)^2 + \frac{1}{ab}(y'_{..} + x)^2 + R \qquad (4\text{-}15)$$

where R includes all terms not involving x. From $dSS_E/dx = 0$, we obtain

$$x = \frac{ay'_{i.} + by'_{.j} - y'_{..}}{(a-1)(b-1)} \qquad (4\text{-}16)$$

as the estimate of the missing observation.

For the data in Table 4-7, we find that $y'_{2.} = 1$, $y'_{.3} = 6$, and $y'_{..} = 17$. Therefore, from Equation 4-16,

$$x \equiv y_{23} = \frac{4(1) + 4(6) - 17}{(3)(3)} = 1.22$$

The usual analysis of variance may now be performed using $y_{23} = 1.22$ and reducing the error degrees of freedom by 1. The analysis of variance is shown in Table 4-8 on the facing page. Compare the results of this approximate analysis with the results obtained for the full data set (Table 4-5).

Table 4-8 Approximate Analysis of Variance for Example 4-1 with One Missing Value

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Type of tip	39.98	3	13.33	17.12	0.0008
Specimens (blocks)	79.53	3	26.51		
Error	6.22	8	0.78		
Total	125.73	14			

If several observations are missing, they may be estimated by writing the error sum of squares as a function of the missing values, differentiating with respect to each missing value, equating the results to zero, and solving the resulting equations. Alternatively, we may use Equation 4-16 iteratively to estimate the missing values. To illustrate the iterative approach, suppose that two values are missing. Arbitrarily estimate the first missing value, and then use this value along with the real data and Equation 4-16 to estimate the second. Now Equation 4-16 can be used to re-estimate the first missing value, and following this, the second can be re-estimated. This process is continued until convergence is obtained. In any missing value problem, the error degrees of freedom are reduced by one for each missing observation.

4-1.4 Estimating Model Parameters and the General Regression Significance Test

If both treatments and blocks are fixed, we may estimate the parameters in the RCBD model by least squares. Recall that the linear statistical model is

$$y_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij} \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \end{cases} \tag{4-17}$$

Applying the rules in Section 3-9.2 for finding the normal equations for an experimental design model, we obtain

$$\begin{aligned}
&\mu: && ab\hat{\mu} + b\hat{\tau}_1 + b\hat{\tau}_2 + \cdots + b\hat{\tau}_a + a\hat{\beta}_1 + a\hat{\beta}_2 + \cdots + a\hat{\beta}_b = y_{..} \\
&\tau_1: && b\hat{\mu} + b\hat{\tau}_1 + \hat{\beta}_1 + \hat{\beta}_2 + \cdots + \hat{\beta}_b = y_{1.} \\
&\tau_2: && b\hat{\mu} + b\hat{\tau}_2 + \hat{\beta}_1 + \hat{\beta}_2 + \cdots + \hat{\beta}_b = y_{2.} \\
&\vdots && \vdots \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \vdots \\
&\tau_a: && b\hat{\mu} + b\hat{\tau}_a + \hat{\beta}_1 + \hat{\beta}_2 + \cdots + \hat{\beta}_b = y_{a.} \\
&\beta_1: && a\hat{\mu} + \hat{\tau}_1 + \hat{\tau}_2 + \cdots + \hat{\tau}_a + a\hat{\beta}_1 = y_{.1} \\
&\beta_2: && a\hat{\mu} + \hat{\tau}_1 + \hat{\tau}_2 + \cdots + \hat{\tau}_a + a\hat{\beta}_2 = y_{.2} \\
&\vdots && \vdots \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \vdots \\
&\beta_b: && a\hat{\mu} + \hat{\tau}_1 + \hat{\tau}_2 + \cdots + \hat{\tau}_a + a\hat{\beta}_b = y_{.b}
\end{aligned} \tag{4-18}$$

Notice that the second through the $(a + 1)$st equations in Equation 4-18 sum to the first normal equation, as do the last b equations. Thus, there are two linear dependencies

in the normal equations, implying that two constraints must be imposed to solve Equation 4-18. The usual constraints are

$$\sum_{i=1}^{a} \hat{\tau}_i = 0 \qquad \sum_{j=1}^{b} \hat{\beta}_j = 0 \tag{4-19}$$

Using these constraints, the normal equations simplify considerably. In fact, they become

$$\begin{aligned} ab\hat{\mu} &= y_{..} \\ b\hat{\mu} + b\hat{\tau}_i &= y_{i.} \qquad i = 1, 2, \ldots, a \\ a\hat{\mu} + a\hat{\beta}_j &= y_{.j} \qquad j = 1, 2, \ldots, b \end{aligned} \tag{4-20}$$

whose solution is

$$\begin{aligned} \hat{\mu} &= \bar{y}_{..} \\ \hat{\tau}_i &= \bar{y}_{i.} - \bar{y}_{..} \qquad i = 1, 2, \ldots, a \\ \hat{\beta}_j &= \bar{y}_{.j} - \bar{y}_{..} \qquad j = 1, 2, \ldots, b \end{aligned} \tag{4-21}$$

Using the solution to the normal equation in Equation 4-21, we may find the estimated or fitted values of y_{ij} as

$$\begin{aligned} \hat{y}_{ij} &= \hat{\mu} + \hat{\tau}_i + \hat{\beta}_j \\ &= \bar{y}_{..} + (\bar{y}_{i.} - \bar{y}_{..}) + (\bar{y}_{.j} - \bar{y}_{..}) \\ &= \bar{y}_{i.} + \bar{y}_{.j} - \bar{y}_{..} \end{aligned}$$

This result was used previously in Equation 4-13 for computing the residuals from a randomized block design.

The general regression significance test can be used to develop the analysis of variance for the randomized complete block design. Using the solution to the normal equations given by Equation 4-21, the reduction in the sum of squares for fitting the full model is

$$\begin{aligned} R(\mu, \tau, \beta) &= \hat{\mu} y_{..} + \sum_{i=1}^{a} \hat{\tau}_i y_{i.} + \sum_{j=1}^{b} \hat{\beta}_j y_{.j} \\ &= \bar{y}_{..} y_{..} + \sum_{i=1}^{a} (\bar{y}_{i.} - \bar{y}_{..}) y_{i.} + \sum_{j=1}^{b} (\bar{y}_{.j} - \bar{y}_{..}) y_{.j} \\ &= \frac{y_{..}^2}{ab} + \sum_{i=1}^{a} \bar{y}_{i.} y_{i.} - \frac{y_{..}^2}{ab} + \sum_{j=1}^{b} \bar{y}_{.j} y_{.j} - \frac{y_{..}^2}{ab} \\ &= \sum_{i=1}^{a} \frac{y_{i.}^2}{b} + \sum_{j=1}^{b} \frac{y_{.j}^2}{a} - \frac{y_{..}^2}{ab} \end{aligned}$$

with $a + b - 1$ degrees of freedom, and the error sum of squares is

$$\begin{aligned} SS_E &= \sum_{i=1}^{a} \sum_{j=1}^{b} y_{ij}^2 - R(\mu, \tau, \beta) \\ &= \sum_{i=1}^{a} \sum_{j=1}^{b} y_{ij}^2 - \sum_{i=1}^{a} \frac{y_{i.}^2}{b} - \sum_{j=1}^{b} \frac{y_{.j}^2}{a} + \frac{y_{..}^2}{ab} \\ &= \sum_{i=1}^{a} \sum_{j=1}^{b} (y_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..})^2 \end{aligned}$$

with $(a-1)(b-1)$ degrees of freedom. Compare this last equation with SS_E in Equation 4-7.

To test the hypothesis $H_0: \tau_i = 0$, the reduced model is

$$y_{ij} = \mu + \beta_j + \epsilon_{ij}$$

which is just a single-factor analysis of variance. By analogy with Equation 3-5, the reduction in the sum of squares for fitting the reduced model is

$$R(\mu, \beta) = \sum_{j=1}^{b} \frac{y_{.j}^2}{a}$$

which has b degrees of freedom. Therefore, the sum of squares due to $\{\tau_i\}$ after fitting μ and $\{\beta_j\}$ is

$$\begin{aligned} R(\tau|\mu, \beta) &= R(\mu, \tau, \beta) - R(\mu, \beta) \\ &= R(\text{Full Model}) - R(\text{Reduced Model}) \\ &= \sum_{i=1}^{a} \frac{y_{i.}^2}{b} + \sum_{j=1}^{b} \frac{y_{.j}^2}{a} - \frac{y_{..}^2}{ab} - \sum_{j=1}^{b} \frac{y_{.j}^2}{a} \\ &= \sum_{i=1}^{a} \frac{y_{i.}^2}{b} - \frac{y_{..}^2}{ab} \end{aligned}$$

which we recognize as the treatment sum of squares with $a-1$ degrees of freedom (Equation 4-10).

The block sum of squares is obtained by fitting the reduced model

$$y_{ij} = \mu + \tau_i + \epsilon_{ij}$$

which is also a single-factor analysis. Again, by analogy with Equation 3-5, the reduction in the sum of squares for fitting this model is

$$R(\mu, \tau) = \sum_{i=1}^{a} \frac{y_{i.}^2}{b}$$

with a degrees of freedom. The sum of squares for blocks $\{\beta_j\}$ after fitting μ and $\{\tau_i\}$ is

$$\begin{aligned} R(\beta|\mu, \tau) &= R(\mu, \tau, \beta) - R(\mu, \tau) \\ &= \sum_{i=1}^{a} \frac{y_{i.}^2}{b} + \sum_{j=1}^{b} \frac{y_{.j}^2}{a} - \frac{y_{..}^2}{ab} - \sum_{i=1}^{a} \frac{y_{i.}^2}{b} \\ &= \sum_{j=1}^{b} \frac{y_{.j}^2}{a} - \frac{y_{..}^2}{ab} \end{aligned}$$

with $b-1$ degrees of freedom, which we have given previously as Equation 4-11.

We have developed the sums of squares for treatments, blocks, and error in the randomized complete block design using the general regression significance test. Although we would not ordinarily use the general regression significance test to actually analyze data in a randomized complete block, the procedure occasionally proves useful in more general randomized block designs, such as those discussed in Section 4-4.

Exact Analysis of the Missing Value Problem

In Section 4-1.3 an approximate procedure for dealing with missing observations in the RCBD was presented. This approximate analysis consists of estimating the missing value so that the error mean square is minimized. It can be shown that the approximate analysis produces a biased mean square for treatments in the sense that $E(MS_{\text{Treatments}})$ is larger than $E(MS_E)$ if the null hypothesis is true. Consequently, too many significant results are reported.

The missing value problem may be analyzed exactly by using the general regression significance test. The missing value causes the design to be **unbalanced**, and because all the treatments do not occur in all blocks, we say that the treatments and blocks are not **orthogonal**. This method of analysis is also used in more general types of randomized block designs; it is discussed further in Section 4-4. Problem 4-26 asks the reader to perform the exact analysis for a randomized complete block design with one missing value.

4-2 THE LATIN SQUARE DESIGN

In Section 4-1 we introduced the randomized complete block design as a design to reduce the residual error in an experiment by removing variability due to a known and controllable nuisance variable. There are several other types of designs that utilize the blocking principle. For example, suppose that an experimenter is studying the effects of five different formulations of a rocket propellant used in aircrew escape systems on the observed burning rate. Each formulation is mixed from a batch of raw material that is only large enough for five formulations to be tested. Furthermore, the formulations are prepared by several operators, and there may be substantial differences in the skills and experience of the operators. Thus, it would seem that there are two nuisance factors to be "averaged out" in the design: batches of raw material and operators. The appropriate design for this problem consists of testing each formulation exactly once in each batch of raw material and for each formulation to be prepared exactly once by each of five operators. The resulting design, shown in Table 4-9, is called a **Latin square design**. Notice that the design is a square arrangement and that the five formulations (or treatments) are denoted by the Latin letters A, B, C, D, and E; hence the name Latin square. We see that both batches of raw material (rows) and operators (columns) are orthogonal to treatments.

The Latin square design is used to eliminate two nuisance sources of variability; that is, it systematically allows blocking in two directions. Thus, the rows and columns actually represent *two restrictions on randomization*. In general, a Latin square for p factors, or a $p \times p$ Latin square, is a square containing p rows and p columns. Each of the

Table 4-9 Latin Square Design for the Rocket Propellant Problem

Batches of Raw Material	Operators				
	1	2	3	4	5
1	$A = 24$	$B = 20$	$C = 19$	$D = 24$	$E = 24$
2	$B = 17$	$C = 24$	$D = 30$	$E = 27$	$A = 36$
3	$C = 18$	$D = 38$	$E = 26$	$A = 27$	$B = 21$
4	$D = 26$	$E = 31$	$A = 26$	$B = 23$	$C = 22$
5	$E = 22$	$A = 30$	$B = 20$	$C = 29$	$D = 31$

resulting p^2 cells contains one of the p letters that corresponds to the treatments, and each letter occurs once and only once in each row and column. Some examples of Latin squares are

4 × 4	5 × 5	6 × 6
A B D C	A D B E C	A D C E B F
B C A D	D A C B E	B A E C F D
C D B A	C B E D A	C E D F A B
D A C B	B E A C D	D C F B E A
	E C D A B	F B A D C E
		E F B A D C

The **statistical model** for a Latin square is

$$y_{ijk} = \mu + \alpha_i + \tau_j + \beta_k + \epsilon_{ijk} \begin{cases} i = 1, 2, \ldots, p \\ j = 1, 2, \ldots, p \\ k = 1, 2, \ldots, p \end{cases} \tag{4-22}$$

where y_{ijk} is the observation in the ith row and kth column for the jth treatment, μ is the overall mean, α_i is the ith row effect, τ_j is the jth treatment effect, β_k is the kth column effect, and ϵ_{ijk} is the random error. Note that this is an **effects model**. The model is completely **additive**; that is, there is no interaction between rows, columns, and treatments. Because there is only one observation in each cell, only two of the three subscripts i, j, and k are needed to denote a particular observation. For example, referring to the rocket propellant problem in Table 4-9, if $i = 2$ and $k = 3$, we automatically find $j = 4$ (formulation D), and if $i = 1$ and $j = 3$ (formulation C), we find $k = 3$. This is a consequence of each treatment appearing exactly once in each row and column.

The analysis of variance consists of partitioning the total sum of squares of the $N = p^2$ observations into components for rows, columns, treatments, and error, for example,

$$SS_T = SS_{\text{Rows}} + SS_{\text{Columns}} + SS_{\text{Treatments}} + SS_E \tag{4-23}$$

with respective degrees of freedom

$$p^2 - 1 = p - 1 + p - 1 + p - 1 + (p - 2)(p - 1)$$

Under the usual assumption that ϵ_{ijk} is NID $(0, \sigma^2)$, each sum of squares on the right-hand side of Equation 4-23 is, upon division by σ^2, an independently distributed chi-square random variable. The appropriate statistic for testing for no differences in treatment means is

$$F_0 = \frac{MS_{\text{Treatments}}}{MS_E}$$

which is distributed as $F_{p-1,(p-2)(p-1)}$ under the null hypothesis. We may also test for no row effect and no column effect by forming the ratio of MS_{Rows} or MS_{Columns} to MS_E. However, because the rows and columns represent restrictions on randomization, these tests may not be appropriate.

The computational procedure for the analysis of variance is shown in Table 4-10 on page 146. From the computational formulas for the sums of squares, we see that the analysis is a simple extension of the RCBD, with the sum of squares resulting from rows obtained from the row totals.

Table 4-10 Analysis of Variance for the Latin Square Design

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Treatments	$SS_{\text{Treatments}} = \frac{1}{p}\sum_{j=1}^{p} y_{\cdot j\cdot}^2 - \frac{y_{\cdots}^2}{N}$	$p-1$	$\frac{SS_{\text{Treatments}}}{p-1}$	$F_0 = \frac{MS_{\text{Treatments}}}{MS_E}$
Rows	$SS_{\text{Rows}} = \frac{1}{p}\sum_{i=1}^{p} y_{i\cdot\cdot}^2 - \frac{y_{\cdots}^2}{N}$	$p-1$	$\frac{SS_{\text{Rows}}}{p-1}$	
Columns	$SS_{\text{Columns}} = \frac{1}{p}\sum_{k=1}^{p} y_{\cdot\cdot k}^2 - \frac{y_{\cdots}^2}{N}$	$p-1$	$\frac{SS_{\text{Columns}}}{p-1}$	
Error	SS_E (by subtraction)	$(p-2)(p-1)$	$\frac{SS_E}{(p-2)(p-1)}$	
Total	$SS_T = \sum_i \sum_j \sum_k y_{ijk}^2 - \frac{y_{\cdots}^2}{N}$	p^2-1		

EXAMPLE 4-3

Consider the rocket propellant problem previously described, where both batches of raw material and operators represent randomization restrictions. The design for this experiment, shown in Table 4-9, is a 5×5 Latin square. After coding by subtracting 25 from each observation, we have the data in Table 4-11. The sums of squares for the total, batches (rows), and operators (columns) are computed as follows:

$$SS_T = \sum_i \sum_j \sum_k y_{ijk}^2 - \frac{y_{\cdots}^2}{N}$$

$$= 680 - \frac{(10)^2}{25} = 676.00$$

$$SS_{\text{Batches}} = \frac{1}{p}\sum_{i=1}^{p} y_{i\cdot\cdot}^2 - \frac{y_{\cdots}^2}{N}$$

$$= \frac{1}{5}[(-14)^2 + 9^2 + 5^2 + 3^2 + 7^2] - \frac{(10)^2}{25} = 68.00$$

$$SS_{\text{Operators}} = \frac{1}{p}\sum_{k=1}^{p} y_{\cdot\cdot k}^2 - \frac{y_{\cdots}^2}{N}$$

$$= \frac{1}{5}[(-18)^2 + 18^2 + (-4)^2 + 5^2 + 9^2] - \frac{(10)^2}{25} = 150.00$$

Table 4-11 Coded Data for the Rocket Propellant Problem

Batches of Raw Material	Operators 1	2	3	4	5	$y_{i\cdot\cdot}$
1	$A = -1$	$B = -5$	$C = -6$	$D = -1$	$E = -1$	-14
2	$B = -8$	$C = -1$	$D = 5$	$E = 2$	$A = 11$	9
3	$C = -7$	$D = 13$	$E = 1$	$A = 2$	$B = -4$	5
4	$D = 1$	$E = 6$	$A = 1$	$B = -2$	$C = -3$	3
5	$E = -3$	$A = 5$	$B = -5$	$C = 4$	$D = 6$	7
$y_{\cdot\cdot k}$	-18	18	-4	5	9	$10 = y_{\cdots}$

Table 4-12 Analysis of Variance for the Rocket Propellant Experiment

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Formulations	330.00	4	82.50	7.73	0.0025
Batches of raw material	68.00	4	17.00		
Operators	150.00	4	37.50		
Error	128.00	12	10.67		
Total	676.00	24			

The totals for the treatments (Latin letters) are

Latin Letter	Treatment Total
A	$y_{.1.} = 18$
B	$y_{.2.} = -24$
C	$y_{.3.} = -13$
D	$y_{.4.} = 24$
E	$y_{.5.} = 5$

The sum of squares resulting from the formulations is computed from these totals as

$$SS_{\text{Formulations}} = \frac{1}{p}\sum_{j=1}^{p} y_{.j.}^2 - \frac{y_{...}^2}{N}$$

$$= \frac{18^2 + (-24)^2 + (-13)^2 + 24^2 + 5^2}{5} - \frac{(10)^2}{25} = 330.00$$

The error sum of squares is found by subtraction:

$$SS_E = SS_T - SS_{\text{Batches}} - SS_{\text{Operators}} - SS_{\text{Formulations}}$$
$$= 676.00 - 68.00 - 150.00 - 330.00 = 128.00$$

The analysis of variance is summarized in Table 4-12. We conclude that there is a significant difference in the mean burning rate generated by the different rocket propellant formulations. There is also an indication that there are differences between operators, so blocking on this factor was a good precaution. There is no strong evidence of a difference between batches of raw material, so it seems that in this particular experiment we were unnecessarily concerned about this source of variability. However, blocking on batches of raw material is usually a good idea.

As in any design problem, the experimenter should investigate the adequacy of the model by inspecting and plotting the residuals. For a Latin square, the residuals are given by

$$e_{ijk} = y_{ijk} - \hat{y}_{ijk}$$
$$= y_{ijk} - \bar{y}_{i..} - \bar{y}_{.j.} - \bar{y}_{..k} + 2\bar{y}_{...}$$

The reader should find the residuals for Example 4-4 and construct appropriate plots.

Table 4-13 Standard Latin Squares and Number of Latin Squares of Various Sizes[a]

Size	3×3	4×4	5×5	6×6	7×7	$p \times p$
Examples of standard squares	$A\ B\ C$ $B\ C\ A$ $C\ A\ B$	$A\ B\ C\ D$ $B\ C\ D\ A$ $C\ D\ A\ B$ $D\ A\ B\ C$	$A\ B\ C\ D\ E$ $B\ A\ E\ C\ D$ $C\ D\ A\ E\ B$ $D\ E\ B\ A\ C$ $E\ C\ D\ B\ A$	$A\ B\ C\ D\ E\ F$ $B\ C\ F\ A\ D\ E$ $C\ F\ B\ E\ A\ D$ $D\ E\ A\ B\ F\ C$ $E\ A\ D\ F\ C\ B$ $F\ D\ E\ C\ B\ A$	$A\ B\ C\ D\ E\ F\ G$ $B\ C\ D\ E\ F\ G\ A$ $C\ D\ E\ F\ G\ A\ B$ $D\ E\ F\ G\ A\ B\ C$ $E\ F\ G\ A\ B\ C\ D$ $F\ G\ A\ B\ C\ D\ E$ $G\ A\ B\ C\ D\ E\ F$	$ABC \ldots P$ $BCD \ldots A$ $CDE \ldots B$ $\vdots$ $PAB \ldots (P-1)$
Number of standard squares	1	4	56	9408	16,942,080	—
Total number of Latin squares	12	576	161,280	818,851,200	61,479,419,904,000	$p!(p-1)! \times$ (number of standard squares)

[a] Some of the information in this table is found in *Statistical Tables for Biological, Agricultural and Medical Research*, 4th edition, by R. A. Fisher and F. Yates, Oliver and Boyd, Edinburgh, 1953. Little is known about the properties of Latin squares larger than 7×7.

A Latin square in which the first row and column consists of the letters written in alphabetical order is called a **standard Latin square**, which is the design used in Example 4-4. A standard Latin square can always be obtained by writing the first row in alphabetical order and then writing each successive row as the row of letters just above shifted one place to the left. Table 4-13 summarizes several important facts about Latin squares and standard Latin squares.

As with any experimental design, the observations in the Latin square should be taken in random order. The proper randomization procedure is to select the particular square employed at random. As we see in Table 4-13, there are a large number of Latin squares of a particular size, so it is impossible to enumerate all the squares and select one randomly. The usual procedure is to select a Latin square from a table of such designs, as in Fisher and Yates (1953), and then arrange the order of the rows, columns, and letters at random. This is discussed more completely in Fisher and Yates (1953).

Occasionally, one observation in a Latin square is missing. For a $p \times p$ Latin square, the missing value may be estimated by

$$y_{ijk} = \frac{p(y'_{i\cdot\cdot} + y'_{\cdot j\cdot} + y'_{\cdot\cdot k}) - 2y'_{\cdot\cdot\cdot}}{(p-2)(p-1)} \tag{4-24}$$

where the primes indicate totals for the row, column, and treatment with the missing value, and $y'_{\cdot\cdot\cdot}$ is the grand total with the missing value.

Latin squares can be useful in situations where the rows and columns represent factors the experimenter actually wishes to study and where there are no randomization restrictions. Thus, three factors (rows, columns, and letters), each at p levels, can be investigated in only p^2 runs. This design assumes that there is no interaction between the factors. More will be said later on the subject of interaction.

Replication of Latin Squares

A disadvantage of small Latin squares is that they provide a relatively small number of error degrees of freedom. For example, a 3×3 Latin square has only two error degrees of freedom, a 4×4 Latin square has only six error degrees of freedom, and so forth. When small Latin squares are used, it is frequently desirable to replicate them to increase the error degrees of freedom.

There are several ways to replicate a Latin square. To illustrate, suppose that the

Table 4-14 Analysis of Variance for a Replicated Latin Square, Case 1

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Treatments	$\frac{1}{np}\sum_{j=1}^{p} y_{.j..}^2 - \frac{y_{....}^2}{N}$	$p-1$	$\frac{SS_{\text{Treatments}}}{p-1}$	$\frac{MS_{\text{Treatments}}}{MS_E}$
Rows	$\frac{1}{np}\sum_{i=1}^{p} y_{i...}^2 - \frac{y_{....}^2}{N}$	$p-1$	$\frac{SS_{\text{Rows}}}{p-1}$	
Columns	$\frac{1}{np}\sum_{k=1}^{p} y_{..k.}^2 - \frac{y_{....}^2}{N}$	$p-1$	$\frac{SS_{\text{Columns}}}{p-1}$	
Replicates	$\frac{1}{p^2}\sum_{l=1}^{n} y_{...l}^2 - \frac{y_{....}^2}{N}$	$n-1$	$\frac{SS_{\text{Replicates}}}{n-1}$	
Error	Subtraction	$(p-1)[n(p+1)-3]$	$\frac{SS_E}{(p-1)[n(p+1)-3]}$	
Total	$\sum\sum\sum\sum y_{ijkl}^2 - \frac{y_{....}^2}{N}$	np^2-1		

5×5 Latin square used in Example 4-4 is replicated n times. This could have been done as follows:

1. Use the same batches and operators in each replicate.
2. Use the same batches but different operators in each replicate (or, equivalently, use the same operators but different batches).
3. Use different batches and different operators.

The analysis of variance depends on the method of replication.

Consider case 1, where the same levels of the row and column blocking factors are used in each replicate. Let y_{ijkl} be the observation in row i, treatment j, column k, and replicate l. There are $N = np^2$ total observations. The analysis of variance is summarized in Table 4-14.

Now consider case 2 and assume that new batches of raw material but the same operators are used in each replicate. Thus, there are now five new rows (in general, p new rows) within each replicate. The analysis of variance is summarized in Table 4-15.

Table 4-15 Analysis of Variance for a Replicated Latin Square, Case 2

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Treatments	$\frac{1}{np}\sum_{j=1}^{p} y_{.j..}^2 - \frac{y_{....}^2}{N}$	$p-1$	$\frac{SS_{\text{Treatments}}}{p-1}$	$\frac{MS_{\text{Treatments}}}{MS_E}$
Rows	$\frac{1}{p}\sum_{l=1}^{n}\sum_{i=1}^{p} y_{i..l}^2 - \sum_{l=1}^{n}\frac{y_{....}^2}{p^2}$	$n(p-1)$	$\frac{SS_{\text{Rows}}}{n(p-1)}$	
Columns	$\frac{1}{np}\sum_{k=1}^{p} y_{..k.}^2 - \frac{y_{....}^2}{N}$	$p-1$	$\frac{SS_{\text{Columns}}}{p-1}$	
Replicates	$\frac{1}{p^2}\sum_{l=1}^{n} y_{...l}^2 - \frac{y_{....}^2}{N}$	$n-1$	$\frac{SS_{\text{Replicates}}}{n-1}$	
Error	Subtraction	$(p-1)(np-1)$	$\frac{SS_E}{(p-1)(np-1)}$	
Total	$\sum_i\sum_j\sum_k\sum_l y_{ijkl}^2 - \frac{y_{....}^2}{N}$	np^2-1		

Table 4-16 Analysis of Variance for a Replicated Latin Square, Case 3

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Treatments	$\frac{1}{np}\sum_{j=1}^{p} y_{j..}^2 - \frac{y_{....}^2}{N}$	$p-1$	$\frac{SS_{\text{Treatments}}}{p-1}$	$\frac{MS_{\text{Treatments}}}{MS_E}$
Rows	$\frac{1}{p}\sum_{l=1}^{n}\sum_{i=1}^{p} y_{i..l}^2 - \sum_{l=1}^{n}\frac{y_{...l}^2}{p^2}$	$n(p-1)$	$\frac{SS_{\text{Rows}}}{n(p-1)}$	
Columns	$\frac{1}{p}\sum_{l=1}^{n}\sum_{k=1}^{p} y_{..kl}^2 - \sum_{l=1}^{n}\frac{y_{...l}^2}{p^2}$	$n(p-1)$	$\frac{SS_{\text{Columns}}}{n(p-1)}$	
Replicates	$\frac{1}{p^2}\sum_{l=1}^{n} y_{...l}^2 - \frac{y_{....}^2}{N}$	$n-1$	$\frac{SS_{\text{Replicates}}}{n-1}$	
Error	Subtraction	$(p-1)[n(p-1)-1]$	$\frac{SS_E}{(p-1)[n(p-1)-1]}$	
Total	$\sum_i\sum_j\sum_k\sum_l y_{ijkl}^2 - \frac{y_{....}^2}{N}$	np^2-1		

Note that the source of variation for the rows really measures the variation between rows within the n replicates.

Finally, consider case 3, where new batches of raw material and new operators are used in each replicate. Now the variation that results from both the rows and columns measures the variation resulting from these factors within the replicates. The analysis of variance is summarized in Table 4-16.

There are other approaches to analyzing replicated Latin squares that allow some interactions between treatments and squares (refer to Problem 4-19).

Crossover Designs and Designs Balanced for Residual Effects

Occasionally, one encounters a problem in which time periods are a factor in the experiment. In general, there are p treatments to be tested in p time periods using np experimental units. For example, a human performance analyst is studying the effect of two replacement fluids on dehydration in 20 subjects. In the first period, half of the subjects (chosen at random) are given fluid A and the other half fluid B. At the end of the period, the response is measured, and a period of time is allowed to pass in which any physiological effect of the fluids is eliminated. Then the experimenter has the subjects who took fluid A take fluid B and those who took fluid B take fluid A. This design is called a **crossover design**. It is analyzed as a set of 10 Latin squares with two rows (time periods) and two treatments (fluid types). The two columns in each of the 10 squares correspond to subjects.

The layout of this design is shown in Figure 4-7. Notice that the rows in the Latin square represent the time periods and the columns represent the subjects. The 10

	Latin Squares																			
	I		II		III		IV		V		VI		VII		VIII		IX		X	
Subject	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Period 1	*A*	*B*	*B*	*A*	*B*	*A*	*A*	*B*	*A*	*B*	*B*	*A*	*A*	*B*	*A*	*B*	*A*	*B*	*A*	*B*
Period 2	*B*	*A*	*A*	*B*	*A*	*B*	*B*	*A*	*B*	*A*	*A*	*B*	*B*	*A*	*B*	*A*	*B*	*A*	*B*	*A*

Figure 4-7 A crossover design.

Table 4-17 Analysis of Variance for the Crossover Design in Figure 4-7

Source of Validation	Degrees of Freedom
Subjects (columns)	19
Periods (rows)	1
Fluids (letters)	1
Error	18
Total	39

subjects who received fluid A first (1, 4, 6, 7, 9, 12, 13, 15, 17, and 19) are randomly determined.

An abbreviated analysis of variance is summarized in Table 4-17. The subject sum of squares is computed as the corrected sum of squares among the 20 subject totals, the period sum of squares is the corrected sum of squares among the rows, and the fluid sum of squares is computed as the corrected sum of squares among the letter totals. For further details of the statistical analysis of these designs, see Cochran and Cox (1957), John (1971), and Anderson and McLean (1974).

It is also possible to employ Latin square type designs for experiments in which the treatments have a **residual effect**—that is, for example, if the data for fluid B in period 2 still reflected some effect of fluid A taken in period 1. Designs balanced for residual effects are discussed in detail by Cochran and Cox (1957) and John (1971).

4-3 THE GRAECO–LATIN SQUARE DESIGN

Consider a $p \times p$ Latin square, and superimpose on it a second $p \times p$ Latin square in which the treatments are denoted by Greek letters. If the two squares when superimposed have the property that each Greek letter appears once and only once with each Latin letter, the two Latin squares are said to be *orthogonal*, and the design obtained is called a **Graeco–Latin square**. An example of a 4×4 Graeco–Latin square is shown in Table 4-18.

The Graeco–Latin square design can be used to control systematically three sources of extraneous variability, that is, to block in *three* directions. The design allows investigation of four factors (rows, columns, Latin letters, and Greek letters), each at p levels in only p^2 runs. Graeco–Latin squares exist for all $p \geq 3$ except $p = 6$.

Table 4-18 4×4 Graeco–Latin Square Design

	Column			
Row	1	2	3	4
1	$A\alpha$	$B\beta$	$C\gamma$	$D\delta$
2	$B\delta$	$A\gamma$	$D\beta$	$C\alpha$
3	$C\beta$	$D\alpha$	$A\delta$	$B\gamma$
4	$D\gamma$	$C\delta$	$B\alpha$	$A\beta$

Table 4-19 Analysis of Variance for a Graeco–Latin Square Design

Source of Variation	Sum of Squares	Degrees of Freedom
Latin letter treatments	$SS_L = \frac{1}{p}\sum_{j=1}^{p} y_{j..}^2 - \frac{y_{....}^2}{N}$	$p - 1$
Greek letter treatments	$SS_G = \frac{1}{p}\sum_{k=1}^{p} y_{..k.}^2 - \frac{y_{....}^2}{N}$	$p - 1$
Rows	$SS_{\text{Rows}} = \frac{1}{p}\sum_{i=1}^{p} y_{i...}^2 - \frac{y_{....}^2}{N}$	$p - 1$
Columns	$SS_{\text{Columns}} = \frac{1}{p}\sum_{l=1}^{p} y_{...l}^2 - \frac{y_{....}^2}{N}$	$p - 1$
Error	SS_E (by subtraction)	$(p - 3)(p - 1)$
Total	$SS_T = \sum_i \sum_j \sum_k \sum_l y_{ijkl}^2 - \frac{y_{....}^2}{N}$	$p^2 - 1$

The statistical model for the Graeco–Latin square design is

$$y_{ijkl} = \mu + \theta_i + \tau_j + \omega_k + \Psi_l + \epsilon_{ijkl} \begin{cases} i = 1, 2, \ldots, p \\ j = 1, 2, \ldots, p \\ k = 1, 2, \ldots, p \\ l = 1, 2, \ldots, p \end{cases} \tag{4-25}$$

where y_{ijkl} is the observation in row i and column l for Latin letter j and Greek letter k, θ_i is the effect of the ith row, τ_j is the effect of Latin letter treatment j, ω_k is the effect of Greek letter treatment k, Ψ_l is the effect of column l, and ϵ_{ijkl} is an NID $(0, \sigma^2)$ random error component. Only two of the four subscripts are necessary to completely identify an observation.

The analysis of variance is very similar to that of a Latin square. Because the Greek letters appear exactly once in each row and column and exactly once with each Latin letter, the factor represented by the Greek letters is orthogonal to rows, columns, and Latin letter treatments. Therefore, a sum of squares due to the Greek letter factor may be computed from the Greek letter totals and the experimental error is further reduced by this amount. The computational details are illustrated in Table 4-19. The null hypotheses of equal row, column, Latin letter, and Greek letter treatments would be tested by dividing the corresponding mean square by mean square error. The rejection region is the upper-tail point of the $F_{p-1,(p-3)(p-1)}$ distribution.

EXAMPLE 4-4

Suppose that in the rocket propellant experiment of Example 4-3 an additional factor, test assemblies, could be of importance. Let there be five test assemblies denoted by the Greek letters α, β, γ, δ, and ϵ. The resulting 5×5 Graeco–Latin square design is shown in Table 4-20 on the facing page.

Notice that, because the totals for batches of raw material (rows), operators (columns) and formulations (Latin letters) are identical to those in Example 4-3, we have

$$SS_{\text{Batches}} = 68.00 \qquad SS_{\text{Operators}} = 150.00 \qquad \text{and} \qquad SS_{\text{Formulations}} = 330.00$$

Table 4-20 Graeco–Latin Square Design for the Rocket Propellant Problem

Batches of Raw Material	Operators 1	2	3	4	5	$y_{i...}$
1	$A\alpha = -1$	$B\gamma = -5$	$C\epsilon = -6$	$D\beta = -1$	$E\delta = -1$	-14
2	$B\beta = -8$	$C\delta = -1$	$D\alpha = 5$	$E\gamma = 2$	$A\epsilon = 11$	9
3	$C\gamma = -7$	$D\epsilon = 13$	$E\beta = 1$	$A\delta = 2$	$B\alpha = -4$	5
4	$D\delta = 1$	$E\alpha = 6$	$A\gamma = 1$	$B\epsilon = -2$	$C\beta = -3$	3
5	$E\epsilon = -3$	$A\beta = 5$	$B\delta = -5$	$C\alpha = 4$	$D\gamma = 6$	7
$y_{...l}$	-18	18	-4	5	9	$10 = y_{....}$

The totals for the test assemblies (Greek letters) are

Greek Letter	Test Assembly Total
α	$y_{..1.} = 10$
β	$y_{..2.} = -6$
γ	$y_{..3.} = -3$
δ	$y_{..4.} = -4$
ϵ	$y_{..5.} = 13$

Thus, the sum of squares due to the test assemblies is

$$SS_{\text{Assemblies}} = \frac{1}{p}\sum_{k=1}^{p} y_{..k.}^2 - \frac{y_{....}^2}{N}$$

$$= \frac{1}{5}[10^2 + (-6)^2 + (-3)^2 + (-4)^2 + 13^2] - \frac{(10)^2}{25} = 62.00$$

The complete analysis of variance is summarized in Table 4-21. Formulations are significantly different at 1 percent. In comparing Tables 4-21 and 4-12, we observe that removing the variability due to test assemblies has decreased the experimental error. However, in decreasing the experimental error, we have also reduced the error degrees of freedom from 12 (in the Latin square design of Example 4-3) to 8. Thus, our estimate of error has fewer degrees of freedom, and the test may be less sensitive.

Table 4-21 Analysis of Variance for the Rocket Propellant Problem

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Formulations	330.00	4	82.50	10.00	0.0033
Batches of raw material	68.00	4	17.00		
Operators	150.00	4	37.50		
Test assemblies	62.00	4	15.50		
Error	66.00	8	8.25		
Total	676.00	24			

The concept of orthogonal pairs of Latin squares forming a Graeco-Latin square can be extended somewhat. A $p \times p$ **hypersquare** is a design in which three or more orthogonal $p \times p$ Latin squares are superimposed. In general, up to $p + 1$ factors could be studied if a complete set of $p - 1$ orthogonal Latin squares is available. Such a design would utilize all $(p + 1)(p - 1) = p^2 - 1$ degrees of freedom, so an independent estimate of the error variance is necessary. Of course, there must be no interactions between the factors when using hypersquares.

4-4 BALANCED INCOMPLETE BLOCK DESIGNS

In certain experiments using randomized block designs, we may not be able to run all the treatment combinations in each block. Situations like this usually occur because of shortages of experimental apparatus or facilities or the physical size of the block. For example, in the hardness testing experiment (Example 4-1), suppose that because of their size each coupon can be used only for testing three tips. Therefore, each tip cannot be tested on each coupon. For this type of problem it is possible to use randomized block designs in which every treatment is not present in every block. These designs are known as **randomized incomplete block designs**.

When all treatment comparisons are equally important, the treatment combinations used in each block should be selected in a balanced manner, that is, so that any pair of treatments occur together the same number of times as any other pair. Thus, a **balanced incomplete block design (BIBD)** is an incomplete block design in which any two treatments appear together an equal number of times. Suppose that there are a treatments and that each block can hold exactly k $(k < a)$ treatments. A balanced incomplete block design may be constructed by taking $\binom{a}{k}$ blocks and assigning a different combination of treatments to each block. Frequently, however, balance can be obtained with fewer than $\binom{a}{k}$ blocks. Tables of BIBDs are given in Fisher and Yates (1953), Davies (1956), and Cochran and Cox (1957).

As an example, suppose that a chemical engineer thinks that the time of reaction for a chemical process is a function of the type of catalyst employed. Four catalysts are currently being investigated. The experimental procedure consists of selecting a batch of raw material, loading the pilot plant, applying each catalyst in a separate run of the pilot plant, and observing the reaction time. Because variations in the batches of raw material may affect the performance of the catalysts, the engineer decides to use batches of raw material as blocks. However, each batch is only large enough to permit three catalysts

Table 4-22 Balanced Incomplete Block Design for Catalyst Experiment

Teratment (Catalyst)	Block (Batch of Raw Material)				
	1	2	3	4	$y_{i.}$
1	73	74	—	71	218
2	—	75	67	72	214
3	73	75	68	—	216
4	75	—	72	75	222
$y_{.j}$	221	224	207	218	$870 = y_{..}$

to be run. Therefore, a randomized incomplete block design must be used. The balanced incomplete block design for this experiment, along with the observations recorded, is shown in Table 4-22 at the bottom of the previous page. The order in which the catalysts are run in each block is randomized.

4-4.1 Statistical Analysis of the BIBD

As usual, we assume that there are a treatments and b blocks. In addition, we assume that each block contains k treatments, that each treatment occurs r times in the design (or is replicated r times), and that there are $N = ar = bk$ total observations. Furthermore, the number of times each pair of treatments appears in the same block is

$$\lambda = \frac{r(k-1)}{a-1}$$

If $a = b$, the design is said to be **symmetric**.

The parameter λ must be an integer. To derive the relationship for λ, consider any treatment, say treatment 1. Because treatment 1 appears in r blocks and there are $k-1$ other treatments in each of those blocks, there are $r(k-1)$ observations in a block containing treatment 1. These $r(k-1)$ observations also have to represent the remaining $a-1$ treatments λ times. Therefore, $\lambda(a-1) = r(k-1)$.

The **statistical model** for the BIBD is

$$y_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij} \tag{4-26}$$

where y_{ij} is the ith observation in the jth block, μ is the overall mean, τ_i is the effect of the ith treatment, β_j is the effect of the jth block, and ϵ_{ij} is the NID $(0, \sigma^2)$ random error component. The total variability in the data is expressed by the total corrected sum of squares:

$$SS_T = \sum_i \sum_j y_{ij}^2 - \frac{y_{..}^2}{N} \tag{4-27}$$

Total variability may be partitioned into

$$SS_T = SS_{\text{Treatments(adjusted)}} + SS_{\text{Blocks}} + SS_E$$

where the sum of squares for treatments is **adjusted** to separate the treatment and the block effects. This adjustment is necessary because each treatment is represented in a different set of r blocks. Thus, differences between unadjusted treatment totals $y_{1.}, y_{2.}, \ldots, y_{a.}$ are also affected by differences between blocks.

The block sum of squares is

$$SS_{\text{Blocks}} = \frac{1}{k}\sum_{j=1}^{b} y_{.j}^2 - \frac{y_{..}^2}{N} \tag{4-28}$$

where $y_{.j}$ is the total in the jth block. SS_{Blocks} has $b-1$ degrees of freedom. The adjusted treatment sum of squares is

$$SS_{\text{Treatments(adjusted)}} = \frac{k\sum_{i=1}^{a} Q_i^2}{\lambda a} \tag{4-29}$$

Table 4-23 Analysis of Variance for the Balanced Incomplete Block Design

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Treatments (adjusted)	$\frac{k\sum Q_i^2}{\lambda a}$	$a-1$	$\frac{SS_{\text{Treatments(adjusted)}}}{a-1}$	$F_0 = \frac{MS_{\text{Treatments(adjusted)}}}{MS_E}$
Blocks	$\frac{1}{k}\sum y_{.j}^2 - \frac{y_{..}^2}{N}$	$b-1$	$\frac{SS_{\text{Blocks}}}{b-1}$	
Error	SS_E (by subtraction)	$N-a-b+1$	$\frac{SS_E}{N-a-b+1}$	
Total	$\sum\sum y_{ij}^2 - \frac{y_{..}^2}{N}$	$N-1$		

where Q_i is the adjusted total for the ith treatment, which is computed as

$$Q_i = y_{i.} - \frac{1}{k}\sum_{j=1}^{b} n_{ij}y_{.j} \qquad i = 1, 2, \ldots, a \tag{4-30}$$

with $n_{ij} = 1$ if treatment i appears in block j and $n_{ij} = 0$ otherwise. The adjusted treatment totals will always sum to zero. $SS_{\text{Treatments(adjusted)}}$ has $a-1$ degrees of freedom. The error sum of squares is computed by subtraction as

$$SS_E = SS_T - SS_{\text{Treatments(adjusted)}} - SS_{\text{Blocks}} \tag{4-31}$$

and has $N-a-b+1$ degrees of freedom.

The appropriate statistic for testing the equality of the treatment effects is

$$F_0 = \frac{MS_{\text{Treatments(adjusted)}}}{MS_E}$$

The analysis of variance is summarized in Table 4-23.

EXAMPLE 4-5

Consider the data in Table 4-22 for the catalyst experiment. This is a BIBD with $a = 4$, $b = 4$, $k = 3$, $r = 3$, $\lambda = 2$, and $N = 12$. The analysis of this data is as follows. The total sum of squares is

$$SS_T = \sum_i \sum_j y_{ij}^2 - \frac{y_{..}^2}{12}$$
$$= 63{,}156 - \frac{(870)^2}{12} = 81.00$$

The block sum of squares is found from Equation 4-28 as

$$SS_{\text{Blocks}} = \frac{1}{3}\sum_{j=1}^{4} y_{.j}^2 - \frac{y_{..}^2}{12}$$
$$= \frac{1}{3}[(221)^2 + (207)^2 + (224)^2 + (218)^2] - \frac{(870)^2}{12} = 55.00$$

Table 4-24 Analysis of Variance for Example 4-5

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Treatments (adjusted for blocks)	22.75	3	7.58	11.66	0.0107
Blocks	55.00	3	—		
Error	3.25	5	0.65		
Total	81.00	11			

To compute the treatment sum of squares adjusted for blocks, we first determine the adjusted treatment totals using Equation 4-30 as

$$Q_1 = (218) - \tfrac{1}{3}(221 + 224 + 218) = -9/3$$
$$Q_2 = (214) - \tfrac{1}{3}(207 + 224 + 218) = -7/3$$
$$Q_3 = (216) - \tfrac{1}{3}(221 + 207 + 224) = -4/3$$
$$Q_4 = (222) - \tfrac{1}{3}(221 + 207 + 218) = 20/3$$

The adjusted sum of squares for treatments is computed from Equation 4-29 as

$$SS_{\text{Treatments(adjusted)}} = \frac{k\sum_{i=1}^{4} Q_i^2}{\lambda a}$$
$$= \frac{3[(-9/3)^2 + (-7/3)^2 + (-4/3)^2 + (20/3)^2]}{(2)(4)} = 22.75$$

The error sum of squares is obtained by subtraction as

$$SS_E = SS_T - SS_{\text{Treatments(adjusted)}} - SS_{\text{Blocks}}$$
$$= 81.00 - 22.75 - 55.00 = 3.25$$

The analysis of variance is shown in Table 4-24. Because the P-value is small, we conclude that the catalyst employed has a significant effect on the time of reaction.

If the factor under study is fixed, tests on individual treatment means may be of interest. If orthogonal contrasts are employed, the contrasts must be made on the **adjusted treatment totals**, the $\{Q_i\}$ rather than the $\{y_{i.}\}$. The contrast sum of squares is

$$SS_C = \frac{k\left(\sum_{i=1}^{a} c_i Q_i\right)^2}{\lambda a \sum_{i=1}^{a} c_i^2}$$

where $\{c_i\}$ are the contrast coefficients. Other multiple comparison methods may be used to compare all the pairs of adjusted treatment effects, which we will find in Section

4-4.2, are estimated by $\hat{\tau}_i = kQ_i/(\lambda a)$. The standard error of an adjusted treatment effect is

$$S = \sqrt{\frac{kMS_E}{\lambda a}} \tag{4-32}$$

In the analysis that we have described the total sum of squares has been partitioned into an adjusted sum of squares for treatments, an unadjusted sum of squares for blocks, and an error sum of squares. Sometimes we would like to assess the block effects. To do this, we require an alternate partitioning of SS_T, that is,

$$SS_T = SS_{\text{Treatments}} + SS_{\text{Blocks(adjusted)}} + SS_E$$

Here $SS_{\text{Treatments}}$ is unadjusted. If the design is symmetric, that is, if $a = b$, a simple formula may be obtained for $SS_{\text{Blocks(adjusted)}}$. The adjusted block totals are

$$Q'_j = y_{.j} - \frac{1}{r}\sum_{i=1}^{a} n_{ij}y_{i.} \qquad j = 1, 2, \ldots, b \tag{4-33}$$

and

$$SS_{\text{Blocks(adjusted)}} = \frac{r\sum_{j=1}^{b}(Q'_j)^2}{\lambda b} \tag{4-34}$$

The BIBD in Example 4-5 is symmetric because $a = b = 4$. Therefore,

$$Q'_1 = (221) - \tfrac{1}{3}(218 + 216 + 222) = 7/3$$
$$Q'_2 = (224) - \tfrac{1}{3}(218 + 214 + 216) = 24/3$$
$$Q'_3 = (207) - \tfrac{1}{3}(214 + 216 + 222) = -31/3$$
$$Q'_4 = (218) - \tfrac{1}{3}(218 + 214 + 222) = 0$$

and

$$SS_{\text{Blocks(adjusted)}} = \frac{3[(7/3)^2 + (24/3)^2 + (-31/3)^2 + (0)^2]}{(2)(4)} = 66.08$$

Also,

$$SS_{\text{Treatments}} = \frac{(218)^2 + (214)^2 + (216)^2 + (222)^2}{3} - \frac{(870)^2}{12} = 11.67$$

Table 4-25 Analysis of Variance for Example 4-5, Including Both Treatments and Blocks

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Treatments (adjusted)	22.75	3	7.58	11.66	0.0107
Treatments (unadjusted)	11.67	3			
Blocks (unadjusted)	55.00	3			
Blocks (adjusted)	66.08	3	22.03	33.90	0.0010
Error	3.25	5	0.65		
Total	81.00	11			

A summary of the analysis of variance for the symmetric BIBD is given in Table 4-25 at the bottom of the previous page. Notice that the sums of squares associated with the mean squares in Table 4-25 do not add to the total sum of squares, that is,

$$SS_T \neq SS_{\text{Treatments(adjusted)}} + SS_{\text{Blocks(adjusted)}} + SS_E$$

This is a consequence of the nonorthogonality of treatments and blocks.

Computer Output

There are several computer packages that will perform the analysis for a balanced incomplete block design. The SAS General Linear Models procedure is one of these, and Minitab, a widely used PC statistics package, is another. The upper portion of Table 4-26 (page 160) is the Minitab General Linear Model output for Example 4-5. Comparing Tables 4-26 and 4-25, we see that Minitab has computed the adjusted treatment sum of squares and the adjusted block sum of squares (they are called "Adj SS" in the Minitab output).

The lower portion of Table 4-26 is a multiple comparison analysis, using the Tukey method. Confidence intervals on the differences in all pairs of means and the Tukey test are displayed. Notice that the Tukey method would lead us to conclude that catalyst 4 is different from the other three.

4-4.2 Least Squares Estimation of the Parameters

Consider estimating the treatment effects for the BIBD model. The least squares normal equations are

$$\begin{aligned}
&\mu: N\hat{\mu} + r\sum_{i=1}^{a}\hat{\tau}_i + k\sum_{j=1}^{b}\hat{\beta}_j = y_{..} \\
&\tau_i: r\hat{\mu} + r\hat{\tau}_i + \sum_{j=1}^{b} n_{ij}\hat{\beta}_j = y_{i.} \qquad i = 1, 2, \ldots, a \\
&\beta_j: k\hat{\mu} + \sum_{i=1}^{a} n_{ij}\hat{\tau}_i + k\hat{\beta}_j = y_{.j} \qquad j = 1, 2, \ldots, b
\end{aligned} \tag{4-35}$$

Imposing $\Sigma\hat{\tau}_i = \Sigma\hat{\beta}_j = 0$, we find that $\hat{\mu} = \bar{y}_{..}$. Furthermore, using the equations for $\{\beta_j\}$ to eliminate the block effects from the equations for $\{\tau_i\}$, we obtain

$$rk\hat{\tau}_i - r\hat{\tau}_i - \sum_{j=1}^{b}\sum_{\substack{p=1 \\ p\neq i}}^{a} n_{ij}n_{pj}\hat{\tau}_p = ky_{i.} - \sum_{j=1}^{b} n_{ij}y_{.j} \tag{4-36}$$

Note that the right-hand side of Equation 4-36 is kQ_i, where Q_i is the ith adjusted treatment total (see Equation 4-29). Now, because $\Sigma_{j=1}^{b} n_{ij}n_{pj} = \lambda$ if $p \neq i$ and $n_{pj}^2 = n_{pj}$ (because $n_{pj} = 0$ or 1), we may rewrite Equation 4-36 as

$$r(k-1)\hat{\tau}_i - \lambda\sum_{\substack{p=1 \\ p\neq i}}^{a}\hat{\tau}_p = kQ_i \qquad i = 1, 2, \ldots, a \tag{4-37}$$

Table 4-26 Minitab (General Linear Model) Analysis for Example 4-5

General Linear Model

```
Factor      Type Levels Values
Catalyst    fixed      4 1 2 3 4
Block       fixed      4 1 2 3 4

Analysis of Variance for Time, using Adjusted SS for Tests

Source     DF     Seq SS     Adj SS     Adj MS        F      P
Catalyst    3     11.667     22.750      7.583    11.67  0.011
Block       3     66.083     66.083     22.028    33.89  0.001
Error       5      3.250      3.250      0.650
Total      11     81.000

Tukey 95.0% Simultaneous Confidence Intervals
Response Variable Time
All Pairwise Comparisons among Levels of Catalyst

Catalyst = 1 subtracted from:

Catalyst    Lower    Center    Upper  ----------+---------+---------+------
2          -2.327    0.2500    2.827   (---------*---------)
3          -1.952    0.6250    3.202    (----------*---------)
4           1.048    3.6250    6.202                (----------*---------)
                                      ----------+---------+---------+------
                                               0.0       2.5       5.0


Catalyst = 2 subtracted from:

Catalyst    Lower    Center    Upper  ----------+---------+---------+------
3          -2.202    0.3750    2.952   (---------*---------)
4           0.798    3.3750    5.952                (----------*---------)
                                      ----------+---------+---------+------
                                               0.0       2.5       5.0


Catalyst = 3 subtracted from:

Catalyst    Lower    Center    Upper  ----------+---------+---------+------
4          0.4228     3.000    5.577              (---------*---------)
                                      ----------+---------+---------+------
                                               0.0       2.5       5.0


Tukey Simultaneous Tests
Response Variable Time
All Pairwise Comparisons among Levels of Catalyst

Catalyst = 1 subtracted from:

Level          Difference       SE of                 Adjusted
Catalyst         of Means  Difference  T-Value   P-Value
2                  0.2500      0.6982   0.3581    0.9825
3                  0.6250      0.6982   0.8951    0.8085
4                  3.6250      0.6982   5.1918    0.0130

Catalyst = 2 subtracted from:

Level          Difference       SE of                 Adjusted
Catalyst         of Means  Difference  T-Value   P-Value
3                  0.3750      0.6982   0.5371    0.9462
4                  3.3750      0.6982   4.8338    0.0175

Catalyst = 3 subtracted from:

Level          Difference       SE of                 Adjusted
Catalyst         of Means  Difference  T-Value   P-Value
4                  3.000       0.6982    4.297    0.0281
```

Finally, note that the constraint $\sum_{i=1}^{a} \hat{\tau}_i = 0$ implies that $\sum_{\substack{p=1 \\ p \neq i}}^{a} \hat{\tau}_p = -\hat{\tau}_i$ and recall that $r(k-1) = \lambda(a-1)$ to obtain

$$\lambda a \hat{\tau}_i = kQ_i \qquad i = 1, 2, \ldots, a \tag{4-38}$$

Therefore, the least squares estimators of the treatment effects in the balanced incomplete block model are

$$\hat{\tau}_i = \frac{kQ_i}{\lambda a} \qquad i = 1, 2, \ldots, a \tag{4-39}$$

As an illustration, consider the BIBD in Example 4.5. Because $Q_1 = -9/3$, $Q_2 = -7/3$, $Q_3 = -4/3$, and $Q_4 = 20/3$, we obtain

$$\hat{\tau}_1 = \frac{3(-9/3)}{(2)(4)} = -9/8 \qquad \hat{\tau}_2 = \frac{3(-7/3)}{(2)(4)} = -7/8$$
$$\hat{\tau}_3 = \frac{3(-4/3)}{(2)(4)} = -4/8 \qquad \hat{\tau}_4 = \frac{3(20/3)}{(2)(4)} = 20/8$$

as we found in Section 4-4.1.

4-4.3 Recovery of Interblock Information in the BIBD

The analysis of the BIBD given in Section 4-4.1 is usually called the **intrablock analysis** because block differences are eliminated and all contrasts in the treatment effects can be expressed as comparisons between observations in the same block. This analysis is appropriate regardless of whether the blocks are fixed or random. Yates (1940) noted that, if the block effects are uncorrelated random variables with zero means and variance σ_β^2, one may obtain additional information about the treatment effects τ_i. Yates called the method of obtaining this additional information the **interblock analysis**.

Consider the block totals $y_{.j}$ as a collection of b observations. The model for these observations [following John (1971)] is

$$y_{.j} = k\mu + \sum_{i=1}^{a} n_{ij}\tau_i + \left(k\beta_j + \sum_{i=1}^{a} \epsilon_{ij}\right) \tag{4-40}$$

where the term in parentheses may be regarded as error. The interblock estimators of μ and τ_i are found by minimizing the least squares function

$$L = \sum_{j=1}^{b} \left(y_{.j} - k\mu - \sum_{i=1}^{a} n_{ij}\tau_i\right)^2$$

This yields the following least squares normal equations:

$$\begin{aligned} &\mu: N\tilde{\mu} + r\sum_{i=1}^{a} \tilde{\tau}_i = y_{..} \\ &\tau_i: kr\tilde{\mu} + r\tilde{\tau}_i + \lambda \sum_{\substack{p=1 \\ p \neq i}}^{a} \tilde{\tau}_p = \sum_{j=1}^{b} n_{ij} y_{.j} \qquad i = 1, 2, \ldots, a \end{aligned} \tag{4-41}$$

where $\tilde{\mu}$ and $\tilde{\tau}_i$ denote the **interblock estimators**. Imposing the constraint $\sum_{i=1}^{a} \hat{\tau}_i = 0$, we obtain the solutions to Equations 4-41 as

$$\tilde{\mu} = \bar{y}_{..} \tag{4-42}$$

$$\tilde{\tau}_i = \frac{\sum_{j=1}^{b} n_{ij} y_{.j} - k r \bar{y}_{..}}{r - \lambda} \qquad i = 1, 2, \ldots, a \tag{4-43}$$

It is possible to show that the interblock estimators $\{\tilde{\tau}_i\}$ and the intrablock estimators $\{\hat{\tau}_i\}$ are uncorrelated.

The interblock estimators $\{\tilde{\tau}_i\}$ can differ from the intrablock estimators $\{\hat{\tau}_i\}$. For example, the interblock estimators for the BIBD in Example 4-5 are computed as follows:

$$\tilde{\tau}_1 = \frac{663 - (3)(3)(72.50)}{3 - 2} = 10.50$$

$$\tilde{\tau}_2 = \frac{649 - (3)(3)(72.50)}{3 - 2} = -3.50$$

$$\tilde{\tau}_3 = \frac{652 - (3)(3)(72.50)}{3 - 2} = -0.50$$

$$\tilde{\tau}_4 = \frac{646 - (3)(3)(72.50)}{3 - 2} = -6.50$$

Note that the values of $\sum_{j=1}^{b} n_{ij} y_{.j}$ were used previously on page 157 in computing the adjusted treatment totals in the intrablock analysis.

Now suppose we wish to combine the interblock and intrablock estimators to obtain a single, unbiased, minimum variance estimate of each τ_i. It is possible to show that both $\hat{\tau}_i$ and $\tilde{\tau}_i$ are unbiased and also that

$$V(\hat{\tau}_i) = \frac{k(a - 1)}{\lambda a^2} \sigma^2 \qquad \text{(intrablock)}$$

and

$$V(\tilde{\tau}_i) = \frac{k(a - 1)}{a(r - \lambda)} (\sigma^2 + k\sigma_\beta^2) \qquad \text{(interblock)}$$

We use a linear combination of the two estimators, say

$$\tau_i^* = \alpha_1 \hat{\tau}_i + \alpha_2 \tilde{\tau}_i \tag{4-44}$$

to estimate τ_i. For this estimation method, the minimum variance unbiased combined estimator τ_i^* should have weights $\alpha_1 = u_1/(u_1 + u_2)$ and $\alpha_2 = u_2/(u_1 + u_2)$, where $u_1 = 1/V(\hat{\tau}_i)$ and $u_2 = 1/V(\tilde{\tau}_i)$. Thus, the optimal weights are inversely proportional to the variances of $\hat{\tau}_i$ and $\tilde{\tau}_i$. This implies that the best combined estimator is

$$\tau_i^* = \frac{\hat{\tau}_i \dfrac{k(a - 1)}{a(r - \lambda)} (\sigma^2 + k\sigma_\beta^2) + \tilde{\tau}_i \dfrac{k(a - 1)}{\lambda a^2} \sigma^2}{\dfrac{k(a - 1)}{\lambda a^2} \sigma^2 + \dfrac{k(a - 1)}{a(r - \lambda)} (\sigma^2 + k\sigma_\beta^2)} \qquad i = 1, 2, \ldots, a$$

which can be simplified to

$$\tau_i^* = \frac{kQ_i(\sigma^2 + k\sigma_\beta^2) + \left(\sum_{j=1}^{b} n_{ij}y_{.j} - kr\bar{y}_{..}\right)\sigma^2}{(r - \lambda)\sigma^2 + \lambda a(\sigma^2 + k\sigma_\beta^2)} \qquad i = 1, 2, \ldots, a \quad (4\text{-}45)$$

Unfortunately, Equation 4-45 cannot be used to estimate the τ_i because the variances σ^2 and σ_β^2 are unknown. The usual approach is to estimate σ^2 and σ_β^2 from the data and replace these parameters in Equation 4-45 by the estimates. The estimate usually taken for σ^2 is the error mean square from the intrablock analysis of variance, or the **intrablock error**. Thus,

$$\hat{\sigma}^2 = MS_E$$

The estimate of σ_β^2 is found from the mean square for blocks adjusted for treatments. In general, for a balanced incomplete block design, this mean square is

$$MS_{\text{Blocks(adjusted)}} = \frac{\left(\frac{k\sum_{i=1}^{a} Q_i^2}{\lambda a} + \sum_{j=1}^{b}\frac{y_{.j}^2}{k} - \sum_{i=1}^{a}\frac{y_{i.}^2}{r}\right)}{(b - 1)} \quad (4\text{-}46)$$

and its expected value [which is derived in Graybill (1961)] is

$$E[MS_{\text{Blocks(adjusted)}}] = \sigma^2 + \frac{a(r - 1)}{b - 1}\sigma_\beta^2$$

Thus, if $MS_{\text{Blocks(adjusted)}} > MS_E$, the estimate of $\hat{\sigma}_\beta^2$ is

$$\hat{\sigma}_\beta^2 = \frac{[MS_{\text{Blocks(adjusted)}} - MS_E](b - 1)}{a(r - 1)} \quad (4\text{-}47)$$

and if $MS_{\text{Blocks(adjusted)}} \leq MS_E$, we set $\hat{\sigma}_\beta^2 = 0$. This results in the combined estimator

$$\tau_i^* = \begin{cases} \dfrac{kQ_i(\hat{\sigma}^2 + k\hat{\sigma}_\beta^2) + \left(\sum_{j=1}^{b} n_{ij}y_{.j} - kr\bar{y}_{..}\right)\hat{\sigma}^2}{(r - \lambda)\hat{\sigma}^2 + \lambda a(\hat{\sigma}^2 + k\hat{\sigma}_\beta^2)}, & \hat{\sigma}_\beta^2 > 0 \quad (4\text{-}48a) \\ \dfrac{y_{i.} - (1/a)y_{..}}{r}, & \hat{\sigma}_\beta^2 = 0 \quad (4\text{-}48b) \end{cases}$$

We now compute the combined estimates for the data in Example 4-5. From Table 4-25 we obtain $\hat{\sigma}^2 = MS_E = 0.65$ and $MS_{\text{Blocks(adjusted)}} = 22.03$. (Note that in computing $MS_{\text{Blocks(adjusted)}}$ we make use of the fact that this is a symmetric design. In general, we must use Equation 4-46.) Because $MS_{\text{Blocks(adjusted)}} > MS_E$, we use Equation 4-47 to estimate σ_β^2 as

$$\hat{\sigma}_\beta^2 = \frac{(22.03 - 0.65)(3)}{4(3 - 1)} = 8.02$$

Therefore, we may substitute $\hat{\sigma}^2 = 0.65$ and $\hat{\sigma}_\beta^2 = 8.02$ into Equation 4-48a to obtain the combined estimates listed below. For convenience, the intrablock and interblock

estimates are also given. In this example, the combined estimates are close to the intrablock estimates because the variance of the interblock estimates is relatively large.

Parameter	Intrablock Estimate	Interblock Estimate	Combined Estimate
τ_1	−1.12	10.50	−1.09
τ_2	−0.88	−3.50	−0.88
τ_3	−0.50	−0.50	−0.50
τ_4	2.50	−6.50	2.47

4-5 PROBLEMS

4-1. A chemist wishes to test the effect of four chemical agents on the strength of a particular type of cloth. Because there might be variability from one bolt to another, the chemist decides to use a randomized block design, with the bolts of cloth considered as blocks. She selects five bolts and applies all four chemicals in random order to each bolt. The resulting tensile strengths follow. Analyze the data from this experiment (use $\alpha = 0.05$) and draw appropriate conclusions.

	Bolt				
Chemical	1	2	3	4	5
1	73	68	74	71	67
2	73	67	75	72	70
3	75	68	78	73	68
4	73	71	75	75	69

4-2. Three different washing solutions are being compared to study their effectiveness in retarding bacteria growth in 5-gallon milk containers. The analysis is done in a laboratory, and only three trials can be run on any day. Because days could represent a potential source of variability, the experimenter decides to use a randomized block design. Observations are taken for four days, and the data are shown here. Analyze the data from this experiment (use $\alpha = 0.05$) and draw conclusions.

	Days			
Solution	1	2	3	4
1	13	22	18	39
2	16	24	17	44
3	5	4	1	22

4-3. Plot the mean tensile strengths observed for each chemical type in Problem 4-1 and compare them to an appropriately scaled t distribution. What conclusions would you draw from this display?

4-4. Plot the average bacteria counts for each solution in Problem 4-2 and compare them to a scaled t distribution. What conclusions can you draw?

4-5. An article in the *Fire Safety Journal* ("The Effect of Nozzle Design on the Stability and Performance of Turbulent Water Jets," Vol. 4, August 1981) describes an experiment in which a shape factor was determined for several different nozzle designs at six levels of

jet efflux velocity. Interest focused on potential differences between nozzle designs, with velocity considered as a nuisance variable. The data are shown below:

Nozzle Design	Jet Efflux Velocity (m/s)					
	11.73	14.37	16.59	20.43	23.46	28.74
1	0.78	0.80	0.81	0.75	0.77	0.78
2	0.85	0.85	0.92	0.86	0.81	0.83
3	0.93	0.92	0.95	0.89	0.89	0.83
4	1.14	0.97	0.98	0.88	0.86	0.83
5	0.97	0.86	0.78	0.76	0.76	0.75

(a) Does nozzle design affect the shape factor? Compare the nozzles with a scatter plot and with an analysis of variance, using $\alpha = 0.05$.
(b) Analyze the residuals from this experiment.
(c) Which nozzle designs are different with respect to shape factor? Draw a graph of the average shape factor for each nozzle type and compare this to a scaled t distribution. Compare the conclusions that you draw from this plot to those from Duncan's multiple range test.

4-6. Consider the ratio control algorithm experiment described in Chapter 3, Section 3.8. The experiment was actually conducted as a randomized block design, where six time periods were selected as the blocks, and all four ratio control algorithms were tested in each time period. The average cell voltage and the standard deviation of voltage (shown in parentheses) for each cell are as follows:

Ratio Control Algorithm	Time Period					
	1	2	3	4	5	6
1	4.93 (0.05)	4.86 (0.04)	4.75 (0.05)	4.95 (0.06)	4.79 (0.03)	4.88 (0.05)
2	4.85 (0.04)	4.91 (0.02)	4.79 (0.03)	4.85 (0.05)	4.75 (0.03)	4.85 (0.02)
3	4.83 (0.09)	4.88 (0.13)	4.90 (0.11)	4.75 (0.15)	4.82 (0.08)	4.90 (0.12)
4	4.89 (0.03)	4.77 (0.04)	4.94 (0.05)	4.86 (0.05)	4.79 (0.03)	4.76 (0.02)

(a) Analyze the average cell voltage data. (Use $\alpha = 0.05$.) Does the choice of ratio control algorithm affect the average cell voltage?
(b) Perform an appropriate analysis on the standard deviation of voltage. (Recall that this is called "pot noise.") Does the choice of ratio control algorithm affect the pot noise?
(c) Conduct any residual analyses that seem appropriate.
(d) Which ratio control algorithm would you select if your objective is to reduce both the average cell voltage *and* the pot noise?

4-7. An aluminum master alloy manufacturer produces grain refiners in ingot form. The company produces the product in four furnaces. Each furnace is known to have its own unique operating characteristics, so any experiment run in the foundry that involves more than one furnace will consider furnaces as a nuisance variable. The process engineers suspect that stirring rate affects the grain size of the product. Each furnace can be run at four

different stirring rates. A randomized block design is run for a particular refiner and the resulting grain size data is shown below:

	Furnace			
Stirring Rate (rpm)	1	2	3	4
5	8	4	5	6
10	14	5	6	9
15	14	6	9	2
20	17	9	3	6

(a) Is there any evidence that stirring rate affects grain size?
(b) Graph the residuals from this experiment on a normal probability plot. Interpret this plot.
(c) Plot the residuals versus furnace and stirring rate. Does this plot convey any useful information?
(d) What should the process engineers recommend concerning the choice of stirring rate and furnace for this particular grain refiner if small grain size is desirable?

4-8. Analyze the data in Problem 4-2 using the general regression significance test.

4-9. Assuming that chemical types and bolts are fixed, estimate the model parameters τ_i and β_j in Problem 4-1.

4-10. Draw an operating characteristic curve for the design in Problem 4-2. Does the test seem to be sensitive to small differences in the treatment effects?

4-11. Suppose that the observation for chemical type 2 and bolt 3 is missing in Problem 4-1. Analyze the problem by estimating the missing value. Perform the exact analysis and compare the results.

4-12. ***Two missing values in a randomized block.*** Suppose that in Problem 4-1 the observations for chemical type 2 and bolt 3 and chemical type 4 and bolt 4 are missing.
(a) Analyze the design by iteratively estimating the missing values, as described in Section 4-1.3.
(b) Differentiate SS_E with respect to the two missing values, equate the results to zero, and solve for estimates of the missing values. Analyze the design using these two estimates of the missing values.
(c) Derive general formulas for estimating two missing values when the observations are in *different* blocks.
(d) Derive general formulas for estimating two missing values when the observations are in the *same* block.

4-13. An industrial engineer is conducting an experiment on eye focus time. He is interested in the effect of the distance of the object from the eye on the focus time. Four different distances are of interest. He has five subjects available for the experiment. Because there may be differences among individuals, he decides to conduct the experiment in a randomized block design. The data obtained follow. Analyze the data from this experiment (use $\alpha = 0.05$) and draw appropriate conclusions.

	Subject				
Distance (ft)	1	2	3	4	5
4	10	6	6	6	6
6	7	6	6	1	6
8	5	3	3	2	5
10	6	4	4	2	3

4-14. The effect of five different ingredients (A, B, C, D, E) on the reaction time of a chemical process is being studied. Each batch of new material is only large enough to permit five runs to be made. Furthermore, each run requires approximately $1\frac{1}{2}$ hours, so only five runs can be made in one day. The experimenter decides to run the experiment as a Latin square so that day and batch effects may be systematically controlled. She obtains the data that follow. Analyze the data from this experiment (use $\alpha = 0.05$) and draw conclusions.

	Day				
Batch	1	2	3	4	5
1	$A = 8$	$B = 7$	$D = 1$	$C = 7$	$E = 3$
2	$C = 11$	$E = 2$	$A = 7$	$D = 3$	$B = 8$
3	$B = 4$	$A = 9$	$C = 10$	$E = 1$	$D = 5$
4	$D = 6$	$C = 8$	$E = 6$	$B = 6$	$A = 10$
5	$E = 4$	$D = 2$	$B = 3$	$A = 8$	$C = 8$

4-15. An industrial engineer is investigating the effect of four assembly methods (A, B, C, D) on the assembly time for a color television component. Four operators are selected for the study. Furthermore, the engineer knows that each assembly method produces such fatigue that the time required for the last assembly may be greater than the time required for the first, regardless of the method. That is, a trend develops in the required assembly time. To account for this source of variability, the engineer uses the Latin square design shown below. Analyze the data from this experiment ($\alpha = 0.05$) and draw appropriate conclusions.

Order of	Operator			
Assembly	1	2	3	4
1	$C = 10$	$D = 14$	$A = 7$	$B = 8$
2	$B = 7$	$C = 18$	$D = 11$	$A = 8$
3	$A = 5$	$B = 10$	$C = 11$	$D = 9$
4	$D = 10$	$A = 10$	$B = 12$	$C = 14$

4-16. Suppose that in Problem 4-14 the observation from batch 3 on day 4 is missing. Estimate the missing value from Equation 4-24, and perform the analysis using the value.

4-17. Consider a $p \times p$ Latin square with rows (α_i), columns (β_k), and treatments (τ_j) fixed. Obtain least squares estimates of the model parameters α_i, β_k, and τ_j.

4-18. Derive the missing value formula (Equation 4-24) for the Latin square design.

4-19. ***Designs involving several Latin squares.*** [See Cochran and Cox (1957), John (1971).] The $p \times p$ Latin square contains only p observations for each treatment. To obtain more replications the experimenter may use several squares, say n. It is immaterial whether the squares used are the same or different. The appropriate model is

$$y_{ijkh} = \mu + \rho_h + \alpha_{i(h)} + \tau_j + \beta_{k(h)} + (\tau\rho)_{jh} + \epsilon_{ijkh} \begin{cases} i = 1, 2, \ldots, p \\ j = 1, 2, \ldots, p \\ k = 1, 2, \ldots, p \\ h = 1, 2, \ldots, n \end{cases}$$

where y_{ijkh} is the observation on treatment j in row i and column k of the hth square. Note that $\alpha_{i(h)}$ and $\beta_{k(h)}$ are the row and column effects in the hth square, ρ_h is the effect of the hth square, and $(\tau\rho)_{jh}$ is the interaction between treatments and squares.

(a) Set up the normal equations for this model, and solve for estimates of the model parameters. Assume that appropriate side conditions on the parameters are $\Sigma_h\hat{\rho}_h = 0$, $\Sigma_i\hat{\alpha}_{i(h)} = 0$, and $\Sigma_k\beta_{k(h)} = 0$ for each h, $\Sigma_j\hat{\tau}_j = 0$, $\Sigma_j(\hat{\tau\rho})_{jh} = 0$ for each h, and $\Sigma_h(\hat{\tau\rho})_{jh} = 0$ for each j.

(b) Write down the analysis of variance table for this design.

4-20. Discuss how the operating characteristics curves in the Appendix may be used with the Latin square design.

4-21. Suppose that in Problem 4-14 the data taken on day 5 were incorrectly analyzed and had to be discarded. Develop an appropriate analysis for the remaining data.

4-22. The yield of a chemical process was measured using five batches of raw material, five acid concentrations, five standing times (A, B, C, D, E), and five catalyst concentrations (α, β, γ, δ, ϵ). The Graeco–Latin square that follows was used. Analyze the data from this experiment (use $\alpha = 0.05$) and draw conclusions.

	Acid Concentration				
Batch	1	2	3	4	5
1	$A\alpha = 26$	$B\beta = 16$	$C\gamma = 19$	$D\delta = 16$	$E\epsilon = 13$
2	$B\gamma = 18$	$C\delta = 21$	$D\epsilon = 18$	$E\alpha = 11$	$A\beta = 21$
3	$C\epsilon = 20$	$D\alpha = 12$	$E\beta = 16$	$A\gamma = 25$	$B\delta = 13$
4	$D\beta = 15$	$E\gamma = 15$	$A\delta = 22$	$B\epsilon = 14$	$C\alpha = 17$
5	$E\delta = 10$	$A\epsilon = 24$	$B\alpha = 17$	$C\beta = 17$	$D\gamma = 14$

4-23. Suppose that in Problem 4-15 the engineer suspects that the workplaces used by the four operators may represent an additional source of variation. A fourth factor, workplace (α, β, γ, δ) may be introduced and another experiment conducted, yielding the Graeco–Latin square that follows. Analyze the data from this experiment (use $\alpha = 0.05$) and draw conclusions.

Order of	Operator			
Assembly	1	2	3	4
1	$C\beta = 11$	$B\gamma = 10$	$D\delta = 14$	$A\alpha = 8$
2	$B\alpha = 8$	$C\delta = 12$	$A\gamma = 10$	$D\beta = 12$
3	$A\delta = 9$	$D\alpha = 11$	$B\beta = 7$	$C\gamma = 15$
4	$D\gamma = 9$	$A\beta = 8$	$C\alpha = 18$	$B\delta = 6$

4-24. Construct a 5×5 hypersquare for studying the effects of five factors. Exhibit the analysis of variance table for this design.

4-25. Consider the data in Problems 4-15 and 4-23. Suppressing the Greek letters in 4-23, analyze the data using the method developed in Problem 4-19.

4-26. Consider the randomized block design with one missing value in Table 4-7. Analyze this data by using the exact analysis of the missing value problem discussed in Section 4-1.4. Compare your results to the approximate analysis of these data given in Table 4-8.

4-27. An engineer is studying the mileage performance characteristics of five types of gasoline additives. In the road test he wishes to use cars as blocks; however, because of a time constraint, he must use an incomplete block design. He runs the balanced design with the

five blocks that follow. Analyze the data from this experiment (use $\alpha = 0.05$) and draw conclusions.

	Car				
Additive	1	2	3	4	5
1		17	14	13	12
2	14	14		13	10
3	12		13	12	9
4	13	11	11	12	
5	11	12	10		8

4-28. Construct a set of orthogonal contrasts for the data in Problem 4-27. Compute the sum of squares for each contrast.

4-29. Seven different hardwood concentrations are being studied to determine their effect on the strength of the paper produced. However, the pilot plant can only produce three runs each day. As days may differ, the analyst uses the balanced incomplete block design that follows. Analyze the data from this experiment (use $\alpha = 0.05$) and draw conclusions.

Hardwood	Days						
Concentration (%)	1	2	3	4	5	6	7
2	114				120		117
4	126	120				119	
6		137	117				134
8	141		129	149			
10		145		150	143		
12			120		118	123	
14				136		130	127

4-30. Analyze the data in Example 4-6 using the general regression significance test.

4-31. Prove that $k\Sigma_{i=1}^{a} Q_i^2/(\lambda a)$ is the adjusted sum of squares for treatments in a BIBD.

4-32. An experimenter wishes to compare four treatments in blocks of two runs. Find a BIBD for this experiment with six blocks.

4-33. An experimenter wishes to compare eight treatments in blocks of four runs. Find a BIBD with 14 blocks and $\lambda = 3$.

4-34. Perform the interblock analysis for the design in Problem 4-27.

4-35. Perform the interblock analysis for the design in Problem 4-29.

4-36. Verify that a BIBD with the parameters $a = 8$, $r = 8$, $k = 4$, and $b = 16$ does not exist.

4-37. Show that the variance of the intrablock estimators $\{\hat{\tau}_i\}$ is $k(a-1)\sigma^2/(\lambda a^2)$.

4-38. ***Extended incomplete block designs.*** Occasionally the block size obeys the relationship $a < k < 2a$. An extended incomplete block design consists of a single replicate of each treatment in each block along with an incomplete block design with $k^* = k - a$. In the balanced case, the incomplete block design will have parameters $k^* = k - a$, $r^* = r - b$, and λ^*. Write out the statistical analysis. (*Hint:* In the extended incomplete block design, we have $\lambda = 2r - b + \lambda^*$.)

5 Introduction to Factorial Designs

5-1 BASIC DEFINITIONS AND PRINCIPLES

Many experiments involve the study of the effects of two or more factors. In general, **factorial designs** are most efficient for this type of experiment. By a factorial design, we mean that in each complete trial or replication of the experiment all possible combinations of the levels of the factors are investigated. For example, if there are a levels of factor A and b levels of factor B, each replicate contains all ab treatment combinations. When factors are arranged in a factorial design, they are often said to be **crossed**.

The effect of a factor is defined to be the change in response produced by a change in the level of the factor. This is frequently called a **main effect** because it refers to the primary factors of interest in the experiment. For example, consider the simple experiment in Figure 5-1. This is a two-factor factorial experiment with both design factors at two levels. We have called these levels "low" and "high" and denoted them "$-$" and "$+$," respectively. The main effect of factor A in this two-level design can be thought of as the difference between the average response at the low level of A and the average response at the high level of A. Numerically, this is

$$A = \frac{40 + 52}{2} - \frac{20 + 30}{2} = 21$$

That is, increasing factor A from the low level to the high level causes an **average response increase** of 21 units. Similarly, the main effect of B is

$$B = \frac{30 + 52}{2} - \frac{20 + 40}{2} = 11$$

If the factors appear at more than two levels, the above procedure must be modified because there are other ways to define the effect of a factor. This point is discussed more completely later.

In some experiments, we may find that the difference in response between the levels of one factor is not the same at all levels of the other factors. When this occurs, there is

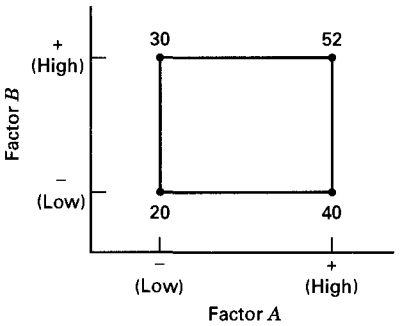


Figure 5-1 A two-factor factorial experiment, with the response (y) shown at the corners.

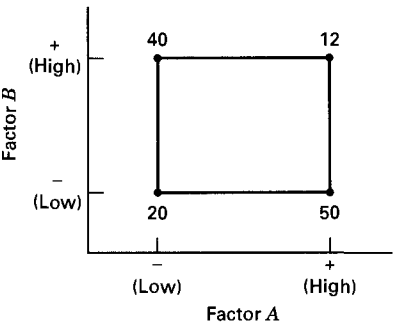


Figure 5-2 A two-factor factorial experiment with interaction.

an **interaction** between the factors. For example, consider the two-factor factorial experiment shown in Figure 5-2. At the low level of factor B (or B^-), the A effect is

$$A = 50 - 20 = 30$$

and at the high level of factor B (or B^+), the A effect is

$$A = 12 - 40 = -28$$

Because the effect of A depends on the level chosen for factor B, we see that there is interaction between A and B. The magnitude of the interaction effect is the average *difference* in these two A effects, or $AB = (-28 - 30)/2 = -29$. Clearly, the interaction is large in this experiment.

These ideas may be illustrated graphically. Figure 5-3 plots the response data in Figure 5-1 against factor A for both levels of factor B. Note that the B^- and B^+ lines are approximately parallel, indicating a lack of interaction between factors A and B. Similarly, Figure 5-4 plots the response data in Figure 5-2. Here we see that the B^- and B^+ lines are not parallel. This indicates an interaction between factors A and B. Graphs such as these are frequently very useful in interpreting significant interactions and in reporting results to nonstatistically trained personnel. However, they should not be utilized as the sole technique of data analysis because their interpretation is subjective and their appearance is often misleading.

There is another way to illustrate the concept of interaction. Suppose that both of our design factors are **quantitative** (such as temperature, pressure, time, etc.). Then a

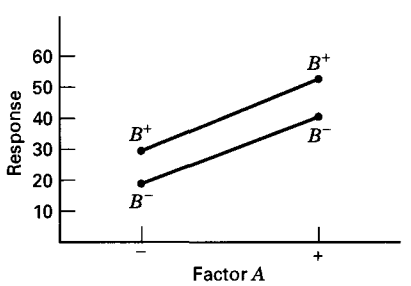


Figure 5-3 A factorial experiment without interaction.

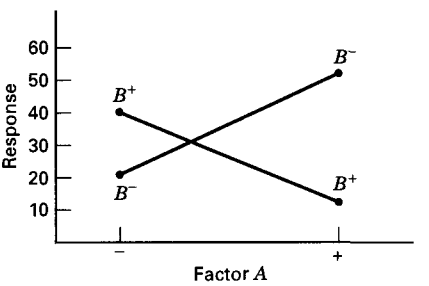


Figure 5-4 A factorial experiment with interaction.

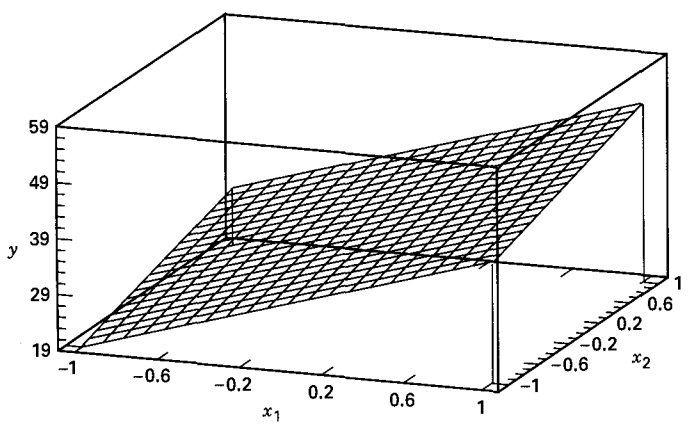
regression model representation of the two-factor factorial experiment could be written as

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \epsilon$$

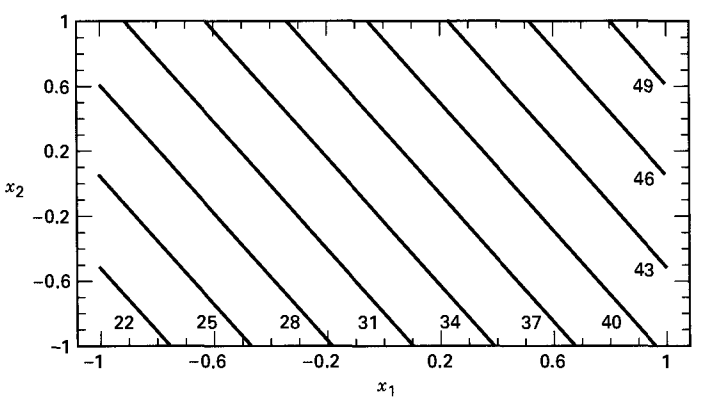
where y is the response, the β's are parameters whose values are to be determined, x_1 is a variable that represents factor A, x_2 is a variable that represents factor B, and ϵ is a random error term. The variables x_1 and x_2 are defined on a **coded scale** from -1 to $+1$ (the low and high levels of A and B), and $x_1 x_2$ represents the interaction between x_1 and x_2.

The parameter estimates in this regression model turn out to be related to the effect estimates. For the experiment shown in Figure 5-1 we found the main effects of A and B to be $A = 21$ and $B = 11$. The estimates of β_1 and β_2 are one-half the value of the corresponding main effect; therefore, $\hat{\beta}_1 = 21/2 = 10.5$ and $\hat{\beta}_2 = 11/2 = 5.5$. The interaction effect in Figure 5-1 is $AB = 1$, so the value of interaction coefficient in the regression model is $\hat{\beta}_{12} = 1/2 = 0.5$. The parameter β_0 is estimated by the average of all four responses, or $\hat{\beta}_0 = (20 + 40 + 30 + 52)/4 = 35.5$. Therefore, the fitted regression model is

$$\hat{y} = 35.5 + 10.5x_1 + 5.5x_2 + 0.5x_1 x_2$$



(*a*) The response surface



(*b*) The contour plot

Figure 5-5 Response surface and contour plot for the model $\hat{y} = 35.5 + 10.5x_1 + 5.5x_2$.

The parameter estimates obtained in the manner for the factorial design with all factors at two levels (− and +) turn out to be **least squares estimates** (more on this later).

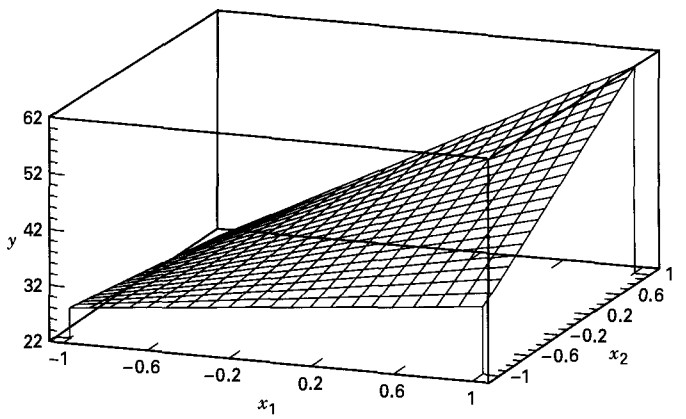
The interaction coefficient ($\hat{\beta}_{12} = 0.5$) is small relative to the main effect coefficients $\hat{\beta}_1$ and $\hat{\beta}_2$. We will take this to mean that interaction is small and can be ignored. Therefore, dropping the term $0.5x_1x_2$ gives us the model

$$\hat{y} = 35.5 + 10.5x_1 + 5.5x_2$$

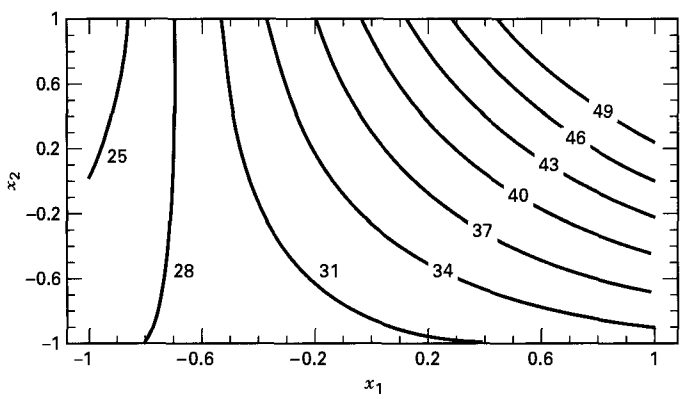
Figure 5-5 presents graphical representations of this model. In Figure 5-5*a* we have a plot of the plane of y-values generated by the various combinations of x_1 and x_2. This three-dimensional graph is called a **response surface plot**. Figure 5-5*b* shows the contour lines of constant response y in the x_1, x_2 plane. Notice that because the response surface is a plane, the contour plot contains parallel straight lines.

Now suppose that the interaction contribution to this experiment was not negligible; that is, the coefficient β_{12} was not small. Figure 5-6 presents the response surface and contour plot for the model

$$\hat{y} = 35.5 + 10.5x_1 + 5.5x_2 + 8x_1x_2$$



(*a*) The response surface



(*b*) The contour plot

Figure 5-6 Response surface and contour plot for the model $\hat{y} = 35.5 + 10.5x_1 + 5.5x_2 + 8x_1x_2$.

(We have let the interaction effect be the average of the two main effects.) Notice that the significant interaction effect "twists" the plane in Figure 5-6*a*. This twisting of the response surface results in curved contour lines of constant response in the x_1, x_2 plane, as shown in Figure 5-6*b*. Thus, **interaction is a form of curvature** in the underlying response surface model for the experiment.

The response surface model for an experiment is extremely important and useful. We will say more about it in Section 5-5 and in subsequent chapters.

Generally, when an interaction is large, the corresponding main effects have little practical meaning. For the experiment in Figure 5-2, we would estimate the main effect of A to be

$$A = \frac{50 + 12}{2} - \frac{20 + 40}{2} = 1$$

which is very small, and we are tempted to conclude that there is no effect due to A. However, when we examine the effects of A at *different levels of factor B*, we see that this is not the case. Factor A has an effect, but it *depends on the level of factor B*. That is, knowledge of the AB interaction is more useful than knowledge of the main effect. A significant interaction will often **mask** the significance of main effects. These points are clearly indicated by the interaction plot in Figure 5-4. In the presence of significant interaction, the experimenter must usually examine the levels of one factor, say A, with levels of the other factors fixed to draw conclusions about the main effect of A.

5-2 THE ADVANTAGE OF FACTORIALS

The advantage of factorial designs can be easily illustrated. Suppose we have two factors A and B, each at two levels. We denote the levels of the factors by A^-, A^+, B^-, and B^+. Information on both factors could be obtained by varying the factors one at a time, as shown in Figure 5-7. The effect of changing factor A is given by $A^+B^- - A^-B^-$ and the effect of changing factor B is given by $A^-B^+ - A^-B^-$. Because experimental error is present, it is desirable to take two observations, say, at each treatment combination and estimate the effects of the factors using average responses. Thus, a total of six observations are required.

If a factorial experiment had been performed, an additional treatment combination,

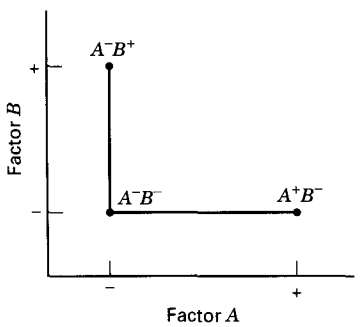


Figure 5-7 A one-factor-at-a-time experiment.

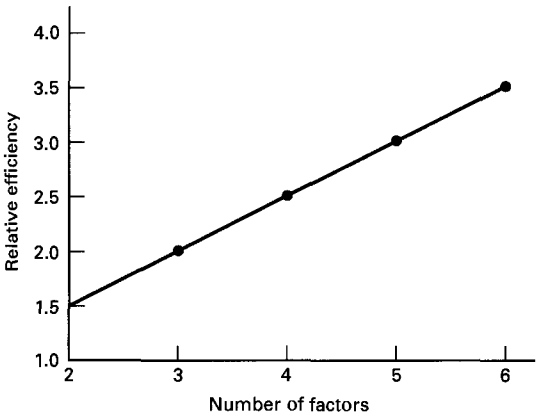


Figure 5-8 Relative efficiency of a factorial design to a one-factor-at-a-time experiment (two factor levels).

A^+B^+, would have been taken. Now, using just *four* observations, two estimates of the A effect can be made: $A^+B^- - A^-B^-$ and $A^+B^+ - A^-B^+$. Similarly, two estimates of the B effect can be made. These two estimates of each main effect could be averaged to produce average main effects that are *just as precise* as those from the single-factor experiment, but only four total observations are required and we would say that the relative efficiency of the factorial design to the one-factor-at-a-time experiment is (6/4) = 1.5. Generally, this relative efficiency will increase as the number of factors increases, as shown in Figure 5-8.

Now suppose interaction is present. If the one-factor-at-a-time design indicated that A^-B^+ and A^+B^- gave better responses than A^-B^-, a logical conclusion would be that A^+B^+ would be even better. However, if interaction is present, this conclusion may be *seriously in error*. For an example, refer to the experiment in Figure 5-2.

In summary, note that factorial designs have several advantages. They are more efficient than one-factor-at-a-time experiments. Furthermore, a factorial design is necessary when interactions may be present to avoid misleading conclusions. Finally, factorial designs allow the effects of a factor to be estimated at several levels of the other factors, yielding conclusions that are valid over a range of experimental conditions.

5-3 THE TWO-FACTOR FACTORIAL DESIGN

5-3.1 An Example

The simplest types of factorial designs involve only two factors or sets of treatments. There are a levels of factor A and b levels of factor B, and these are arranged in a factorial design; that is, each replicate of the experiment contains all ab treatment combinations. In general, there are n replicates.

As an example of a factorial design involving two factors, an engineer is designing a battery for use in a device that will be subjected to some extreme variations in temperature. The only design parameter that he can select at this point is the plate material for the battery, and he has three possible choices. When the device is manufactured and is shipped to the field, the engineer has no control over the temperature extremes that

Table 5-1 Life (in hours) Data for the Battery Design Example

Material Type	Temperature (°F)					
	15		70		125	
1	130	155	34	40	20	70
	74	180	80	75	82	58
2	150	188	136	122	25	70
	159	126	106	115	58	45
3	138	110	174	120	96	104
	168	160	150	139	82	60

the device will encounter, and he knows from experience that temperature will probably affect the effective battery life. However, temperature can be controlled in the product development laboratory for the purposes of a test.

The engineer decides to test all three plate materials at three temperature levels—15, 70, and 125°F—because these temperature levels are consistent with the product end-use environment. Four batteries are tested at each combination of plate material and temperature, and all 36 tests are run in random order. The experiment and the resulting observed battery life data are given in Table 5-1.

In this problem the engineer wants to answer the following questions:

1. What effects do material type and temperature have on the life of the battery?
2. Is there a choice of material that would give *uniformly long life regardless of temperature*?

This last question is particularly important. It may be possible to find a material alternative that is not greatly affected by temperature. If this is so, the engineer can make the battery **robust** to temperature variation in the field. This is an example of using statistical experimental design for **robust product design**, a very important engineering problem.

This design is a specific example of the general case of a two-factor factorial. To pass to the general case, let y_{ijk} be the observed response when factor A is at the ith level ($i = 1, 2, \ldots, a$) and factor B is at the jth level ($j = 1, 2, \ldots, b$) for the kth replicate ($k = 1, 2, \ldots, n$). In general, a two-factor factorial experiment will appear as in Table 5-2. The order in which the abn observations are taken is selected at random so that this design is a **completely randomized design**.

Table 5-2 General Arrangement for a Two-Factor Factorial Design

		Factor B			
		1	2	$\cdots$	b
Factor A	1	$y_{111}, y_{112}, \ldots, y_{11n}$	$y_{121}, y_{122}, \ldots, y_{12n}$		$y_{1b1}, y_{1b2}, \ldots, y_{1bn}$
	2	$y_{211}, y_{212}, \ldots, y_{21n}$	$y_{221}, y_{222}, \ldots, y_{22n}$		$y_{2b1}, y_{2b2}, \ldots, y_{2bn}$
	$\vdots$				
	a	$y_{a11}, y_{a12}, \ldots, y_{a1n}$	$y_{a21}, y_{a22}, \ldots, y_{a2n}$		$y_{ab1}, y_{ab2}, \ldots, y_{abn}$

The observations in a factorial experiment can be described by a model. There are several ways to write the model for a factorial experiment. The **effects model** is

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases} \tag{5-1}$$

where μ is the overall mean effect, τ_i is the effect of the ith level of the row factor A, β_j is the effect of the jth level of column factor B, $(\tau\beta)_{ij}$ is the effect of the interaction between τ_i and β_j, and ϵ_{ijk} is a random error component. Both factors are assumed to be **fixed**, and the treatment effects are defined as deviations from the overall mean, so $\sum_{i=1}^{a} \tau_i = 0$ and $\sum_{j=1}^{b} \beta_j = 0$. Similarly, the interaction effects are fixed and are defined such that $\sum_{i=1}^{a} (\tau\beta)_{ij} = \sum_{j=1}^{b} (\tau\beta)_{ij} = 0$. Because there are n replicates of the experiment, there are abn total observations.

Another possible model for a factorial experiment is the **means model**

$$y_{ijk} = \mu_{ij} + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases}$$

where the mean of the ijth cell is

$$\mu_{ij} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij}$$

We could also use a **regression model** as in Section 5-1. Regression models are particularly useful when one or more of the factors in the experiment are quantitative. Throughout most of this chapter we will use the effects model (Equation 5-1) with reference to the regression model in Section 5-5.

In the two-factor factorial, both row and column factors (or treatments), A and B, are of equal interest. Specifically, we are interested in **testing hypotheses** about the equality of row treatment effects, say

$$\begin{aligned} &H_0: \tau_1 = \tau_2 = \cdots = \tau_a = 0 \\ &H_1: \text{at least one } \tau_i \neq 0 \end{aligned} \tag{5-2a}$$

and the equality of column treatment effects, say

$$\begin{aligned} &H_0: \beta_1 = \beta_2 = \cdots = \beta_b = 0 \\ &H_1: \text{at least one } \beta_j \neq 0 \end{aligned} \tag{5-2b}$$

We are also interested in determining whether row and column treatments *interact*. Thus, we also wish to test

$$\begin{aligned} &H_0: (\tau\beta)_{ij} = 0 \qquad \text{for all } i, j \\ &H_1: \text{at least one } (\tau\beta)_{ij} \neq 0 \end{aligned} \tag{5-2c}$$

We now discuss how these hypotheses are tested using a **two-factor analysis of variance.**

5-3.2 Statistical Analysis of the Fixed Effects Model

Let $y_{i..}$ denote the total of all observations under the ith level of factor A, $y_{.j.}$ denote the total of all observations under the jth level of factor B, $y_{ij.}$ denote the total of all obser-

vations in the ijth cell, and $y_{...}$ denote the grand total of all the observations. Define $\bar{y}_{i..}$, $\bar{y}_{.j.}$, $\bar{y}_{ij.}$, and $\bar{y}_{...}$ as the corresponding row, column, cell, and grand averages. Expressed mathematically,

$$\begin{aligned} y_{i..} &= \sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk} & \bar{y}_{i..} &= \frac{y_{i..}}{bn} & i &= 1, 2, \ldots, a \\ y_{.j.} &= \sum_{i=1}^{a}\sum_{k=1}^{n} y_{ijk} & \bar{y}_{.j.} &= \frac{y_{.j.}}{an} & j &= 1, 2, \ldots, b \\ y_{ij.} &= \sum_{k=1}^{n} y_{ijk} & \bar{y}_{ij.} &= \frac{y_{ij.}}{n} & i &= 1, 2, \ldots, a \\ & & & & j &= 1, 2, \ldots, b \\ y_{...} &= \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk} & \bar{y}_{...} &= \frac{y_{...}}{abn} \end{aligned} \tag{5-3}$$

The **total corrected sum of squares** may be written as

$$\begin{aligned} \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} (y_{ijk} - \bar{y}_{...})^2 &= \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} [(\bar{y}_{i..} - \bar{y}_{...}) + (\bar{y}_{.j.} - \bar{y}_{...}) \\ &\quad + (\bar{y}_{ij.} - \bar{y}_{i..} - \bar{y}_{.j.} + \bar{y}_{...}) + (y_{ijk} - \bar{y}_{ij.})]^2 \\ &= bn\sum_{i=1}^{a} (\bar{y}_{i..} - \bar{y}_{...})^2 + an\sum_{j=1}^{b} (\bar{y}_{.j.} - \bar{y}_{...})^2 \\ &\quad + n\sum_{i=1}^{a}\sum_{j=1}^{b} (\bar{y}_{ij.} - \bar{y}_{i..} - \bar{y}_{.j.} + \bar{y}_{...})^2 \\ &\quad + \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} (y_{ijk} - \bar{y}_{ij.})^2 \end{aligned} \tag{5-4}$$

because the six cross-products on the right-hand side are zero. Notice that the total sum of squares has been partitioned into a sum of squares due to "rows," or factor A, (SS_A); a sum of squares due to "columns," or factor B, (SS_B); a sum of squares due to the interaction between A and B, (SS_{AB}); and a sum of squares due to error, (SS_E). From the last component on the right-hand side of Equation 5-4, we see that there must be at least two replicates ($n \geq 2$) to obtain an error sum of squares.

We may write Equation 5-4 symbolically as

$$SS_T = SS_A + SS_B + SS_{AB} + SS_E \tag{5-5}$$

The number of degrees of freedom associated with each sum of squares is

Effect	Degrees of Freedom
A	$a - 1$
B	$b - 1$
AB interaction	$(a - 1)(b - 1)$
Error	$ab(n - 1)$
Total	$abn - 1$

We may justify this allocation of the $abn - 1$ total degrees of freedom to the sums of squares as follows: The main effects A and B have a and b levels, respectively; therefore they have $a - 1$ and $b - 1$ degrees of freedom as shown. The interaction degrees of freedom are simply the number of degrees of freedom for cells (which is $ab - 1$) minus the number of degrees of freedom for the two main effects A and B; that is, $ab - 1 - (a - 1) - (b - 1) = (a - 1)(b - 1)$. Within each of the ab cells, there are $n - 1$ degrees of freedom between the n replicates; thus there are $ab(n - 1)$ degrees of freedom for error. Note that the number of degrees of freedom on the right-hand side of Equation 5-5 adds to the total number of degrees of freedom.

Each sum of squares divided by its degrees of freedom is a **mean square**. The expected values of the mean squares are

$$E(MS_A) = E\left(\frac{SS_A}{a-1}\right) = \sigma^2 + \frac{bn\sum_{i=1}^{a}\tau_i^2}{a-1}$$

$$E(MS_B) = E\left(\frac{SS_B}{b-1}\right) = \sigma^2 + \frac{an\sum_{j=1}^{b}\beta_j^2}{b-1}$$

$$E(MS_{AB}) = E\left(\frac{SS_{AB}}{(a-1)(b-1)}\right) = \sigma^2 + \frac{n\sum_{i=1}^{a}\sum_{j=1}^{b}(\tau\beta)_{ij}^2}{(a-1)(b-1)}$$

and

$$E(MS_E) = E\left(\frac{SS_E}{ab(n-1)}\right) = \sigma^2$$

Notice that if the null hypotheses of no row treatment effects, no column treatment effects, and no interaction are true, then MS_A, MS_B, MS_{AB}, and MS_E all estimate σ^2. However, if there are differences between row treatment effects, say, then MS_A will be larger than MS_E. Similarly, if there are column treatment effects or interaction present, then the corresponding mean squares will be larger than MS_E. Therefore, to test the significance of both main effects and their interaction, simply divide the corresponding mean square by the error mean square. Large values of this ratio imply that the data do not support the null hypothesis.

If we assume that the model (Equation 5-1) is adequate and that the error terms ϵ_{ijk} are normally and independently distributed with constant variance σ^2, then each of the ratios of mean squares MS_A/MS_E, MS_B/MS_E, and MS_{AB}/MS_E are distributed as F with $a - 1$, $b - 1$, and $(a - 1)(b - 1)$ numerator degrees of freedom, respectively, and $ab(n - 1)$ denominator degrees of freedom,[1] and the critical region would be the upper tail of the F distribution. The test procedure is usually summarized in an **analysis of variance table**, as shown in Table 5-3 on the next page.

Computationally, we usually employ a statistical software package to conduct an

[1] The F test may be viewed as an approximation to a randomization test, as noted previously.

Table 5-3 The Analysis of Variance Table for the Two-Factor Factorial, Fixed Effects Model

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
A treatments	SS_A	$a - 1$	$MS_A = \frac{SS_A}{a - 1}$	$F_0 = \frac{MS_A}{MS_E}$
B treatments	SS_B	$b - 1$	$MS_B = \frac{SS_B}{b - 1}$	$F_0 = \frac{MS_B}{MS_E}$
Interaction	SS_{AB}	$(a - 1)(b - 1)$	$MS_{AB} = \frac{SS_{AB}}{(a - 1)(b - 1)}$	$F_0 = \frac{MS_{AB}}{MS_E}$
Error	SS_E	$ab(n - 1)$	$MS_E = \frac{SS_E}{ab(n - 1)}$	
Total	SS_T	$abn - 1$		

analysis of variance. However, manual computing formulas for the sums of squares in Equation 5-5 may be obtained easily. The total sum of squares is computed as usual by

$$SS_T = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{k=1}^{n} y_{ijk}^2 - \frac{y_{...}^2}{abn} \tag{5-6}$$

The sums of squares for the main effects are

$$SS_A = \frac{1}{bn} \sum_{i=1}^{a} y_{i..}^2 - \frac{y_{...}^2}{abn} \tag{5-7}$$

and

$$SS_B = \frac{1}{an} \sum_{j=1}^{b} y_{.j.}^2 - \frac{y_{...}^2}{abn} \tag{5-8}$$

It is convenient to obtain the SS_{AB} in two stages. First we compute the sum of squares between the ab cell totals, which is called the sum of squares due to "subtotals":

$$SS_{\text{Subtotals}} = \frac{1}{n} \sum_{i=1}^{a} \sum_{j=1}^{b} y_{ij.}^2 - \frac{y_{...}^2}{abn}$$

This sum of squares also contains SS_A and SS_B. Therefore, the second step is to compute SS_{AB} as

$$SS_{AB} = SS_{\text{Subtotals}} - SS_A - SS_B \tag{5-9}$$

We may compute SS_E by subtraction as

$$SS_E = SS_T - SS_{AB} - SS_A - SS_B \tag{5-10}$$

or

$$SS_E = SS_T - SS_{\text{Subtotals}}$$

EXAMPLE 5-1

The Battery Design Experiment

Table 5-4 presents the effective life (in hours) observed in the battery design example described in Section 5-3.1. The row and column totals are shown in the margins of the table and the circled numbers are the cell totals.

Table 5-4 Life Data (in hours) for the Battery Design Experiment

Material Type	Temperature (°F) 15		70		125		$y_{i..}$
1	130 74	155 180 (539)	34 80	40 75 (229)	20 82	70 58 (230)	998
2	150 159	188 126 (623)	136 106	122 115 (479)	25 58	70 45 (198)	1300
3	138 168	110 160 (576)	174 150	120 139 (583)	96 82	104 60 (342)	1501
$y_{.j.}$	1738		1291		770		$3799 = y_{...}$

The sums of squares are computed as follows:

$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk}^2 - \frac{y_{...}^2}{abn}$$

$$= (130)^2 + (155)^2 + (74)^2 + \cdots + (60)^2 - \frac{(3799)^2}{36} = 77{,}646.97$$

$$SS_{\text{Material}} = \frac{1}{bn}\sum_{i=1}^{a} y_{i..}^2 - \frac{y_{...}^2}{abn}$$

$$= \frac{1}{(3)(4)}[(998)^2 + (1300)^2 + (1501)^2] - \frac{(3799)^2}{36} = 10{,}683.72$$

$$SS_{\text{Temperature}} = \frac{1}{an}\sum_{j=1}^{b} y_{.j.}^2 - \frac{y_{...}^2}{abn}$$

$$= \frac{1}{(3)(4)}[(1738)^2 + (1291)^2 + (770)^2] - \frac{(3799)^2}{36} = 39{,}118.72$$

$$SS_{\text{Interaction}} = \frac{1}{n}\sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij.}^2 - \frac{y_{...}^2}{abn} - SS_{\text{Material}} - SS_{\text{Temperature}}$$

$$= \frac{1}{4}[(539)^2 + (229)^2 + \cdots + (342)^2] - \frac{(3799)^2}{36} - 10{,}683.72$$
$$- 39{,}118.72 = 9613.78$$

and

$$SS_E = SS_T - SS_{\text{Material}} - SS_{\text{Temperature}} - SS_{\text{Interaction}}$$
$$= 77{,}646.97 - 10{,}683.72 - 39{,}118.72 - 9613.78 = 18{,}230.75$$

The analysis of variance is shown in Table 5-5 on the next page. Because $F_{0.05,4,27} = 2.73$, we conclude that there is a significant interaction between material types and temperature. Furthermore, $F_{0.05,2,27} = 3.35$, so the main effects of material type and temperature are also significant. Table 5-5 also shows the P-values for the test statistics.

To assist in interpreting the results of this experiment, it is helpful to construct a graph of the average responses at each treatment combination. This graph is shown in Figure 5-9 at the bottom the the next page. The significant interaction is indicated by the lack of parallelism of the lines. In general, longer life is attained at low temperature, regardless of material type. Changing from low to intermediate temperature, battery life

Table 5-5 Analysis of Variance for Battery Life Data

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Material types	10,683.72	2	5,341.86	7.91	0.0020
Temperature	39,118.72	2	19,559.36	28.97	0.0001
Interaction	9,613.78	4	2,403.44	3.56	0.0186
Error	18,230.75	27	675.21		
Total	77,646.97	35			

with material type 3 actually *increases*, whereas it decreases for types 1 and 2. From intermediate to high temperature, battery life decreases for material types 2 and 3 and is essentially unchanged for type 1. Material type 3 seems to give the best results if we want less loss of effective life as the temperature changes.

Multiple Comparisons

When the analysis of variance indicates that row or column means differ, it is usually of interest to make comparisons between the individual row or column means to discover the specific differences. The multiple comparison methods discussed in Chapter 3 are useful in this regard.

We now illustrate the use of Tukey's test on the battery life data in Example 5-1. Note that in this experiment, interaction is significant. When interaction is significant, comparisons between the means of one factor (e.g., A) may be obscured by the AB interaction. One approach to this situation is to fix factor B at a specific level and apply Tukey's test to the means of factor A at that level. To illustrate, suppose that in Example 5-1 we are interested in detecting differences among the means of the three material types. Because interaction is significant, we make this comparison at just one level of temperature, say level 2 (70°F). We assume that the best estimate of the error variance is the MS_E from the analysis of variance table, utilizing the assumption that the experimental error variance is the same over all treatment combinations.

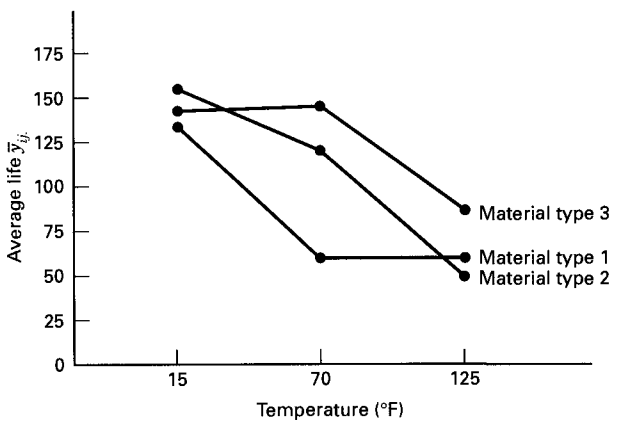


Figure 5-9 Material type–temperature plot for Example 5-1.

The three material type averages at 70°F arranged in ascending order are

$$\begin{aligned} \bar{y}_{12.} &= 57.25 \quad \text{(material type 1)} \\ \bar{y}_{22.} &= 119.75 \quad \text{(material type 2)} \\ \bar{y}_{32.} &= 145.75 \quad \text{(material type 3)} \end{aligned}$$

and

$$\begin{aligned} T_{0.05} &= q_{0.05}(3, 27)\sqrt{\frac{MS_E}{n}} \\ &= 3.50\sqrt{\frac{675.21}{4}} \\ &= 45.47 \end{aligned}$$

where we obtained $q_{0.05}(3, 27) \simeq 3.50$ by interpolation in Appendix Table VIII. The pairwise comparisons yield

$$\begin{aligned} &3 \text{ vs. } 1: \quad 145.75 - 57.25 = 88.50 > T_{0.05} = 45.47 \\ &3 \text{ vs. } 2: \quad 145.75 - 119.75 = 26.00 < T_{0.05} = 45.47 \\ &2 \text{ vs. } 1: \quad 119.75 - 57.25 = 62.50 > T_{0.05} = 45.47 \end{aligned}$$

This analysis indicates that at the temperature level 70°F, the mean battery life is the same for material types 2 and 3, and that the mean battery life for material type 1 is significantly lower in comparison to both types 2 and 3.

If interaction is significant, the experimenter could compare *all ab* cell means to determine which ones differ significantly. In this analysis, differences between cell means include interaction effects as well as both main effects. In Example 5-1, this would give 36 comparisons between all possible pairs of the nine cell means.

Computer Output

Figure 5-10 (on the next page) presents condensed computer output from Design-Expert for the battery life data in Example 5-1. Note that

$$\begin{aligned} SS_{\text{Model}} &= SS_{\text{Material}} + SS_{\text{Temperature}} + SS_{\text{Interaction}} \\ &= 10{,}683.72 + 39{,}118.72 + 9613.78 \\ &= 59{,}416.22 \end{aligned}$$

and that

$$R^2 = \frac{SS_{\text{Model}}}{SS_{\text{Total}}} = \frac{59{,}416.22}{77{,}646.97} = 0.7652$$

That is, about 77 percent of the variability in the battery life is explained by the plate material in the battery, the temperature, and the material type—temperature interaction. The residuals from the fitted model are also displayed on the computer output. We now show how to use these residuals in model adequacy checking.

Response: Life in hours
ANOVA for Selected Factorial Model
Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Model	59416.22	8	7427.03	11.00	<0.0001	significant
A	*10683.72*	*2*	*5341.86*	*7.91*	*0.0020*	
B	*39118.72*	*2*	*19559.36*	*28.97*	*<0.0001*	
AB	*9613.78*	*4*	*2403.44*	*3.56*	*0.0186*	
Residual	18230.75	27	675.21			
Lack of Fit	*0.000*	*0*				
Pure Error	*18230.75*	*27*	*675.21*			
Cor Total	77646.97	35				

Std. Dev.	25.98	R-Squared	0.7652
Mean	105.53	Adj R-Squared	0.6956
C.V.	24.62	Pred R-Squared	0.5826
PRESS	32410.22	Adeq Precision	8.178

Diagnostics Case Statistics

Standard Order	Actual Value	Predicted Value	Residual	Leverage	Student Residual	Cook's Distance	Outlier t
1	130.00	134.75	−4.75	0.250	−0.211	0.002	−0.207
2	74.00	134.75	−60.75	0.250	−2.700	0.270	−3.100
3	155.00	134.75	20.25	0.250	0.900	0.030	0.897
4	180.00	134.75	45.25	0.250	2.011	0.150	2.140
5	150.00	155.75	−5.75	0.250	−0.256	0.002	−0.251
6	159.00	155.75	3.25	0.250	0.144	0.001	0.142
7	188.00	155.75	32.25	0.250	1.433	0.076	1.463
8	126.00	155.75	−29.75	0.250	−1.322	0.065	−1.341
9	138.00	144.00	−6.00	0.250	−0.267	0.003	−0.262
10	168.00	144.00	24.00	0.250	1.066	0.042	1.069
11	110.00	144.00	−34.00	0.250	−1.511	0.085	−1.550
12	160.00	144.00	16.00	0.250	0.711	0.019	0.704
13	34.00	57.25	−23.25	0.250	−1.033	0.040	−1.035
14	80.00	57.25	22.75	0.250	1.011	0.038	1.011
15	40.00	57.25	−17.25	0.250	−0.767	0.022	−0.761
16	75.00	57.25	17.75	0.250	0.789	0.023	0.783
17	136.00	119.75	16.25	0.250	0.722	0.019	0.716
18	106.00	119.75	−13.75	0.250	−0.611	0.014	−0.604
19	122.00	119.75	2.25	0.250	0.100	0.000	0.098
20	115.00	119.75	−4.75	0.250	−0.211	0.002	−0.207
21	174.00	145.75	28.25	0.250	1.255	0.058	1.269
22	150.00	145.75	4.25	0.250	0.189	0.001	0.185
23	120.00	145.75	−25.75	0.250	−1.144	0.048	−1.151
24	139.00	145.75	−6.75	0.250	−0.300	0.003	−0.295
25	20.00	57.50	−37.50	0.250	−1.666	0.103	−1.726
26	82.00	57.50	24.50	0.250	1.089	0.044	1.093
27	70.00	57.50	12.50	0.250	0.555	0.011	0.548
28	58.00	57.50	0.50	0.250	0.022	0.000	0.022
29	25.00	49.50	−24.50	0.250	−1.089	0.044	−1.093
30	58.00	49.50	8.50	0.250	0.378	0.005	0.372
31	70.00	49.50	20.50	0.250	0.911	0.031	0.908
32	45.00	49.50	−4.50	0.250	−0.200	0.001	−0.196
33	96.00	85.50	10.50	0.250	0.467	0.008	0.460
34	82.00	85.50	−3.50	0.250	−0.156	0.001	−0.153
35	104.00	85.50	18.50	0.250	0.822	0.025	0.817
36	60.00	85.50	−25.50	0.250	−1.133	0.048	−1.139

Figure 5-10 Design-Expert output for Example 5-1.

5-3.3 Model Adequacy Checking

Before the conclusions from the analysis of variance are adopted, the adequacy of the underlying model should be checked. As before, the primary diagnostic tool is **residual analysis**. The residuals for the two-factor factorial model are

$$e_{ijk} = y_{ijk} - \hat{y}_{ijk} \tag{5-11}$$

and because the fitted value $\hat{y}_{ijk} = \bar{y}_{ij.}$ (the average of the observations in the ijth cell), Equation 5-11 becomes

$$e_{ijk} = y_{ijk} - \bar{y}_{ij.} \tag{5-12}$$

The residuals from the battery life data in Example 5-1 are shown in the Design-Expert computer output (Figure 5-10) and in Table 5-6. The normal probability plot of these residuals (Figure 5-11, page 186) does not reveal anything particularly troublesome, although the largest negative residual (-60.75 at 15°F for material type 1) does stand out somewhat from the others. The standardized value of this residual is $-60.75/\sqrt{675.21} = -2.34$, and this is the only residual whose absolute value is larger than 2.

Figure 5-12 (page 186) plots the residuals versus the fitted values $\hat{y}_{ijk}$. This plot indicates a mild tendency for the variance of the residuals to increase as the battery life increases. Figures 5-13 and 5-14 (page 187) plot the residuals versus material types and temperature, respectively. Both plots indicate mild inequality of variance, with the treatment combination of 15°F and material type 1 possibly having larger variance than the others.

From Table 5-6 we see that the 15°F–material type 1 cell contains both extreme residuals (-60.75 and 45.25). These two residuals are primarily responsible for the inequality of variance detected in Figures 5-12, 5-13, and 5-14. Reexamination of the data does not reveal any obvious problem, such as an error in recording, so we accept these responses as legitimate. It is possible that this particular treatment combination produces slightly more erratic battery life than the others. The problem, however, is not severe enough to have a dramatic impact on the analysis and conclusions.

5-3.4 Estimating the Model Parameters

The parameters in the effects model for two-factor factorial

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \epsilon_{ijk} \tag{5-13}$$

Table 5-6 Residuals for Example 5-1

Material Type	Temperature (°F)					
	15		70		125	
1	−4.75	20.25	−23.25	−17.25	−37.50	12.50
	−60.75	45.25	22.75	17.75	24.50	0.50
2	−5.75	32.25	16.25	2.25	−24.50	20.50
	3.25	−29.75	−13.75	−4.75	8.50	−4.50
3	−6.00	−34.00	28.25	−25.75	10.50	18.50
	24.00	16.00	4.25	−6.75	−3.50	−25.50

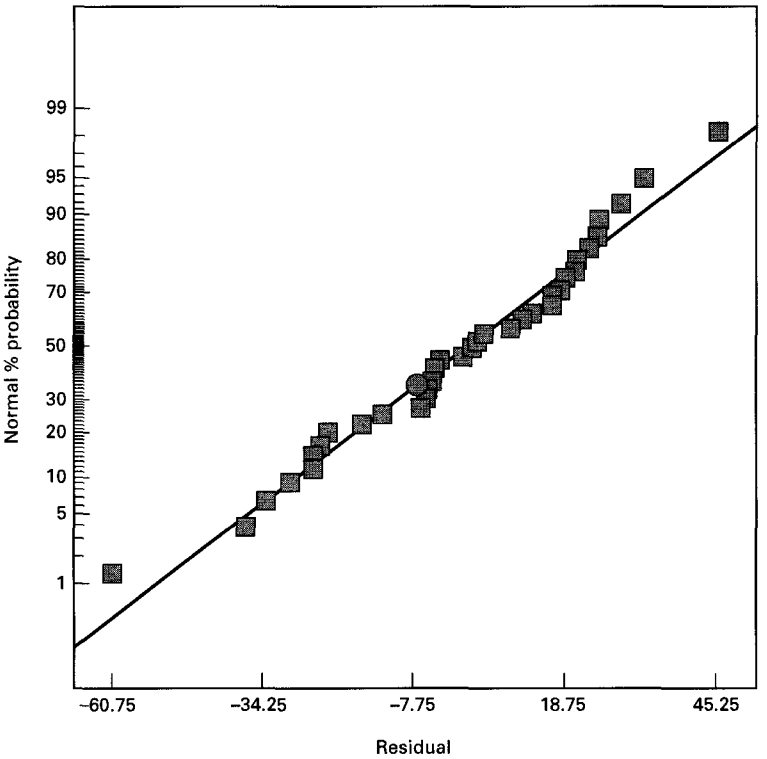


Figure 5-11 Normal probability plot of residuals for Example 5-1.

may be estimated by least squares. Because the model has $1 + a + ab$ parameters to be estimated, there are $1 + a + b + ab$ normal equations. Using the method of Section 3-9, it is not difficult to show that the normal equations are

$$\mu: abn\hat{\mu} + bn \sum_{i=1}^{a} \hat{\tau}_i + an \sum_{j=1}^{b} \hat{\beta}_j + n \sum_{i=1}^{a} \sum_{j=1}^{b} (\widehat{\tau\beta})_{ij} = y_{...} \tag{5-14a}$$

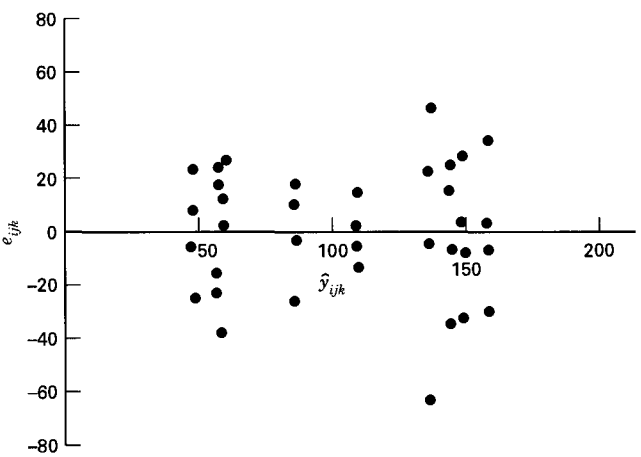


Figure 5-12 Plot of residuals versus $\hat{y}_{ijk}$ for Example 5-1.

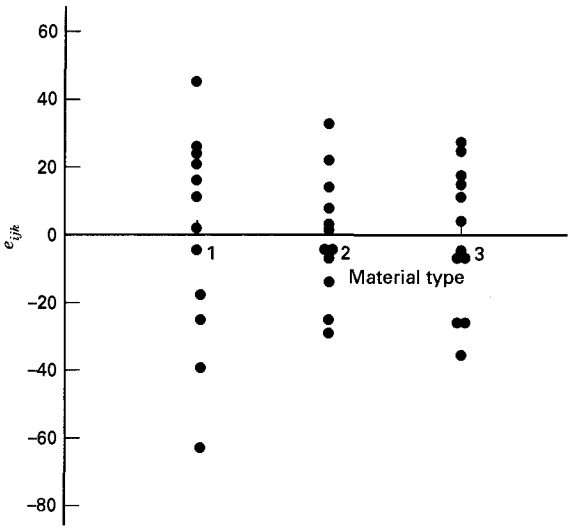


Figure 5-13 Plot of residuals versus material type for Example 5-1.

$$\tau_i\text{: } bn\hat{\mu} + bn\hat{\tau}_i + n\sum_{j=1}^{b}\hat{\beta}_j + n\sum_{j=1}^{b}\widehat{(\tau\beta)}_{ij} = y_{i..} \qquad i = 1, 2, \ldots, a \qquad \text{(5-14b)}$$

$$\beta_j\text{: } an\hat{\mu} + n\sum_{i=1}^{a}\hat{\tau}_i + an\hat{\beta}_j + n\sum_{i=1}^{a}\widehat{(\tau\beta)}_{ij} = y_{.j.} \qquad j = 1, 2, \ldots, b \qquad \text{(5-14c)}$$

$$(\tau\beta)_{ij}\text{: } n\hat{\mu} + n\hat{\tau}_i + n\hat{\beta}_j + n\widehat{(\tau\beta)}_{ij} = y_{ij.} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \end{cases} \qquad \text{(5-14d)}$$

For convenience, we have shown the parameter corresponding to each normal equation on the left in Equations 5-14.

The effects model (Equation 5-13) is an overparameterized model. Notice that the a

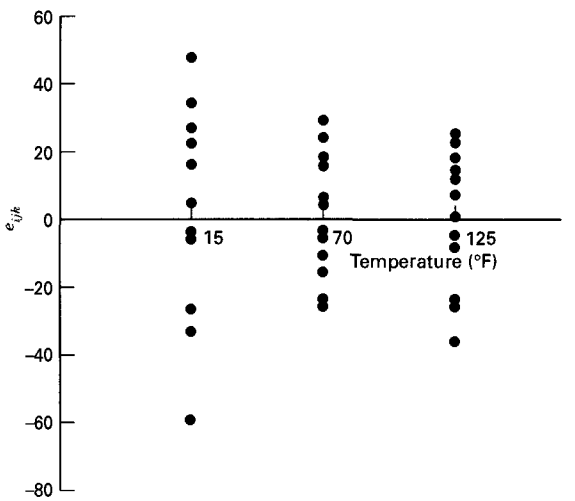


Figure 5-14 Plot of residuals versus temperature for Example 5-1.

equations in Equation 5-14b sum to Equation 5-14a and that the b equations of Equation 5-14c sum to Equation 5-14a. Also summing Equation 5-14d over j for a particular i will give Equation 5-14b, and summing Equation 5-14d over i for a particular j will give Equation 5-14c. Therefore, there are $a + b + 1$ **linear dependencies** in this system of equations and no unique solution will exist. In order to obtain a solution, we impose the constraints

$$\sum_{i=1}^{a} \hat{\tau}_i = 0 \tag{5-15a}$$

$$\sum_{j=1}^{b} \hat{\beta}_j = 0 \tag{5-15b}$$

$$\sum_{i=1}^{a} (\widehat{\tau\beta})_{ij} = 0 \qquad j = 1, 2, \ldots, b \tag{5-15c}$$

and

$$\sum_{j=1}^{b} (\widehat{\tau\beta})_{ij} = 0 \qquad i = 1, 2, \ldots, a \tag{5-15d}$$

Equations 5-15a and 5-15b constitute two constraints, whereas Equations 5-15c and 5-15d form $a + b - 1$ independent constraints. Therefore, we have $a + b + 1$ total constraints, the number needed.

Applying these constraints, the normal equations (Equations 5-14) simplify considerably, and we obtain the solution

$$\begin{aligned} \hat{\mu} &= \bar{y}_{...} \\ \hat{\tau}_i &= \bar{y}_{i..} - \bar{y}_{...} \qquad i = 1, 2, \ldots, a \\ \hat{\beta}_j &= \bar{y}_{.j.} - \bar{y}_{...} \qquad j = 1, 2, \ldots, b \\ (\widehat{\tau\beta})_{ij} &= \bar{y}_{ij.} - \bar{y}_{i..} - \bar{y}_{.j.} + \bar{y}_{...} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \end{cases} \end{aligned} \tag{5-16}$$

Notice the considerable intuitive appeal of this solution to the normal equations. Row treatment effects are estimated by the row average minus the grand average; column treatments are estimated by the column average minus the grand average; and the ijth interaction is estimated by the ijth cell average minus the grand average, the ith row effect, and the jth column effect.

Using Equation 5-16, we may find the **fitted value** y_{ijk} as

$$\begin{aligned} \hat{y}_{ijk} &= \hat{\mu} + \hat{\tau}_i + \hat{\beta}_j + (\widehat{\tau\beta})_{ij} \\ &= \bar{y}_{...} + (\bar{y}_{i..} - \bar{y}_{...}) + (\bar{y}_{.j.} - \bar{y}_{...}) \\ &\quad + (\bar{y}_{ij.} - \bar{y}_{i..} - \bar{y}_{.j.} + \bar{y}_{...}) \\ &= \bar{y}_{ij.} \end{aligned}$$

That is, the kth observation in the ijth cell is estimated by the average of the n observations in that cell. This result was used in Equation 5-12 to obtain the residuals for the two-factor factorial model.

Because constraints (Equations 5-15) have been used to solve the normal equations, the model parameters are not uniquely estimated. However, certain important **functions** of the model parameters *are* estimable, that is, uniquely estimated regardless of the constraint chosen. An example is $\tau_i - \tau_u + (\overline{\tau\beta})_{i.} - (\overline{\tau\beta})_{u.}$, which might be thought of as the "true" difference between the ith and the uth levels of factor A. Notice that the true difference between the levels of any main effect includes an "average" interaction

effect. It is this result that disturbs the tests on main effects in the presence of interaction, as noted earlier. In general, any function of the model parameters that is a linear combination of the left-hand side of the normal equations is **estimable**. This property was also noted in Chapter 3 when we were discussing the single-factor model. For more information, see the supplemental text material for this chapter.

5-3.5 Choice of Sample Size

The operating characteristic curves in Appendix Chart V can be used to assist the experimenter in determining an appropriate sample size (number of replicates, n) for a two-factor factorial design. The appropriate value of the parameter Φ^2 and the numerator and denominator degrees of freedom are shown in Table 5-7.

A very effective way to use these curves is to find the smallest value of Φ^2 corresponding to a specified difference between any two treatment means. For example, if the difference in any two row means is D, then the minimum value of Φ^2 is

$$\Phi^2 = \frac{nbD^2}{2a\sigma^2} \tag{5-17}$$

whereas if the difference in any two column means is D, then the minimum value of Φ^2 is

$$\Phi^2 = \frac{naD^2}{2b\sigma^2} \tag{5-18}$$

Finally, the minimum value of Φ^2 corresponding to a difference of D between any two interaction effects is

$$\Phi^2 = \frac{nD^2}{2\sigma^2[(a-1)(b-1)+1]} \tag{5-19}$$

To illustrate the use of these equations, consider the battery life data in Example 5-1. Suppose that before running the experiment we decide that the null hypothesis should be rejected with a high probability if the difference in mean battery life between any two

Table 5-7 Operating Characteristic Curve Parameters for Chart V of the Appendix for the Two-Factor Factorial, Fixed Effects Model

Factor	Φ^2	Numerator Degrees of Freedom	Denominator Degrees of Freedom
A	$\dfrac{bn\sum_{i=1}^{a}\tau_i^2}{a\sigma^2}$	$a-1$	$ab(n-1)$
B	$\dfrac{an\sum_{j=1}^{b}\beta_j^2}{b\sigma^2}$	$b-1$	$ab(n-1)$
AB	$\dfrac{n\sum_{i=1}^{a}\sum_{j=1}^{b}(\tau\beta)_{ij}^2}{\sigma^2[(a-1)(b-1)+1]}$	$(a-1)(b-1)$	$ab(n-1)$

temperatures is as great as 40 hours. Thus $D = 40$, and if we assume that the standard deviation of battery life is approximately 25, then Equation 5-18 gives

$$\Phi^2 = \frac{naD^2}{2b\sigma^2} = \frac{n(3)(40)^2}{2(3)(25)^2} = 1.28n$$

as the minimum value of Φ^2. Assuming that $\alpha = 0.05$, we can now use Appendix Table V to construct the following display:

n	Φ^2	Φ	ν_1 = Numerator Degrees of Freedom	ν_2 = Error Degrees of Freedom	β
2	2.56	1.60	2	9	0.45
3	3.84	1.96	2	18	0.18
4	5.12	2.26	2	27	0.06

Note that $n = 4$ replicates give a β risk of about 0.06, or approximately a 94 percent chance of rejecting the null hypothesis if the difference in mean battery life at any two temperature levels is as large as 40 hours. Thus, we conclude that four replicates are enough to provide the desired sensitivity as long as our estimate of the standard deviation of battery life is not seriously in error. If in doubt, the experimenter could repeat the above procedure with other values of σ to determine the effect of misestimating this parameter on the sensitivity of the design.

5-3.6 The Assumption of No Interaction in a Two-Factor Model

Occasionally, an experimenter feels that a **two-factor model without interaction** is appropriate, say

$$y_{ijk} = \mu + \tau_i + \beta_j + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases} \tag{5-20}$$

We should be very careful in dispensing with the interaction terms, however, because the presence of significant interaction can have a dramatic impact on the interpretation of the data.

The statistical analysis of a two-factor factorial model without interaction is straightforward. Table 5-8 presents the analysis of the battery life data from Example 5-1, as-

Table 5-8 Analysis of Variance for Battery Life Data Assuming No Interaction

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Material types	10,683.72	2	5,341.86	5.95
Temperature	39,118.72	2	19,559.36	21.78
Error	27,844.52	31	898.21	
Total	77,646.96	35		

suming that the no-interaction model (Equation 5-20) applies. As noted previously, both main effects are significant. However, as soon as a residual analysis is performed for these data, it becomes clear that the no-interaction model is inadequate. For the two-factor model without interaction, the fitted values are $\hat{y}_{ijk} = \bar{y}_{i..} + \bar{y}_{.j.} - \bar{y}_{...}$. A plot of $\bar{y}_{ij.} - \hat{y}_{ijk}$ (the cell averages minus the fitted value for that cell) versus the fitted value $\hat{y}_{ijk}$ is shown in Figure 5-15. Now the quantities $\bar{y}_{ij.} - \hat{y}_{ijk}$ may be viewed as the differences between the observed cell means and the estimated cell means assuming no interaction. Any pattern in these quantities is suggestive of the presence of interaction. Figure 5-15 shows a distinct pattern as the quantities $\bar{y}_{ij.} - \hat{y}_{ijk}$ move from positive to negative to positive to negative again. This structure is the result of interaction between material types and temperature.

5-3.7 One Observation per Cell

Occasionally, one encounters a two-factor experiment with only a **single replicate**, that is, only one observation per cell. If there are two factors and only one observation per cell, the effects model is

$$y_{ij} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \epsilon_{ij} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \end{cases} \tag{5-21}$$

The analysis of variance for this situation is shown in Table 5-9 on the next page, assuming that both factors are fixed.

From examining the expected mean squares, we see that the error variance σ^2 is *not estimable*; that is, the two-factor interaction effect $(\tau\beta)_{ij}$ and the experimental error cannot be separated in any obvious manner. Consequently, there are no tests on main effects unless the interaction effect is zero. If there is no interaction present, then $(\tau\beta)_{ij} = 0$ for all i and j, and a plausible model is

$$y_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \end{cases} \tag{5-22}$$

If the model (Equation 5-22) is appropriate, then the residual mean square in Table 5-9 is an unbiased estimator of σ^2, and the main effects may be tested by comparing MS_A and MS_B to MS_{Residual}.

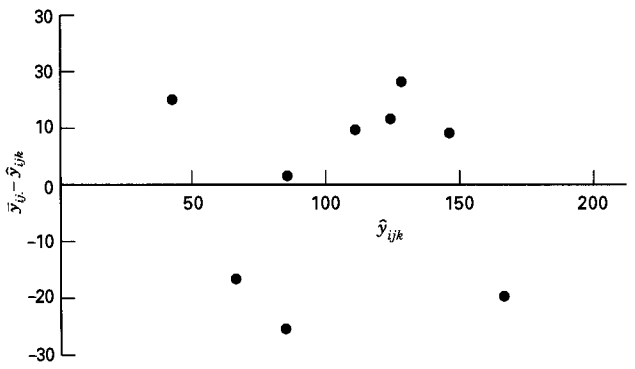


Figure 5-15 Plot of $\bar{y}_{ij.} - \hat{y}_{ijk}$ versus $\hat{y}_{ijk}$, battery life data.

Table 5-9 Analysis of Variance for a Two-Factor Model, One Observation per Cell

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	Expected Mean Square
Rows (A)	$\sum_{i=1}^{a} \frac{y_{i.}^2}{b} - \frac{y_{..}^2}{ab}$	$a - 1$	MS_A	$\sigma^2 + \frac{b \sum \tau_i^2}{a - 1}$
Columns (B)	$\sum_{j=1}^{b} \frac{y_{.j}^2}{a} - \frac{y_{..}^2}{ab}$	$b - 1$	MS_B	$\sigma^2 + \frac{a \sum \beta_j^2}{b - 1}$
Residual or AB	Subtraction	$(a - 1)(b - 1)$	MS_{Residual}	$\sigma^2 + \frac{\sum \sum (\tau\beta)_{ij}^2}{(a - 1)(b - 1)}$
Total	$\sum_{i=1}^{a} \sum_{j=1}^{b} y_{ij}^2 - \frac{y_{..}^2}{ab}$	$ab - 1$		

A test developed by Tukey (1949a) is helpful in determining if interaction is present. The procedure assumes that the interaction term is of a particularly simple form, namely,

$$(\tau\beta)_{ij} = \gamma\tau_i\beta_j$$

where γ is an unknown constant. By defining the interaction term this way, we may use a regression approach to test the significance of the interaction term. The test partitions the residual sum of squares into a single-degree-of-freedom component due to nonadditivity (interaction) and a component for error with $(a - 1)(b - 1) - 1$ degrees of freedom. Computationally, we have

$$SS_N = \frac{\left[\sum_{i=1}^{a} \sum_{j=1}^{b} y_{ij} y_{i.} y_{.j} - y_{..}\left(SS_A + SS_B + \frac{y_{..}^2}{ab}\right)\right]^2}{abSS_ASS_B} \tag{5-23}$$

with one degree of freedom, and

$$SS_{\text{Error}} = SS_{\text{Residual}} - SS_N \tag{5-24}$$

with $(a - 1)(b - 1) - 1$ degrees of freedom. To test for the presence of interaction, we compute

$$F_0 = \frac{SS_N}{SS_{\text{Error}}/[(a - 1)(b - 1) - 1]} \tag{5-25}$$

If $F_0 > F_{\alpha,1,(a-1)(b-1)-1}$, the hypothesis of no interaction must be rejected.

EXAMPLE 5-2

The impurity present in a chemical product is affected by two factors—pressure and temperature. The data from a single replicate of a factorial experiment are shown in Table 5-10. The sums of squares are

$$SS_A = \frac{1}{b} \sum_{i=1}^{a} y_{i.}^2 - \frac{y_{..}^2}{ab}$$

$$= \frac{1}{5}[23^2 + 13^2 + 8^2] - \frac{44^2}{(3)(5)} = 23.33$$

Table 5-10 Impurity Data for Example 5-2

Temperature (°F)	Pressure 25	30	35	40	45	$y_{i.}$
100	5	4	6	3	5	23
125	3	1	4	2	3	13
150	1	1	3	1	2	8
$y_{.j}$	9	6	13	6	10	$44 = y_{..}$

$$SS_B = \frac{1}{a}\sum_{j=1}^{b} y_{.j}^2 - \frac{y_{..}^2}{ab}$$
$$= \frac{1}{3}[9^2 + 6^2 + 13^2 + 6^2 + 10^2] - \frac{44^2}{(3)(5)} = 11.60$$
$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij}^2 - \frac{y_{..}^2}{ab}$$
$$= 166 - 129.07 = 36.93$$

and

$$SS_{\text{Residual}} = SS_T - SS_A - SS_B$$
$$= 36.93 - 23.33 - 11.60 = 2.00$$

The sum of squares for nonadditivity is computed from Equation 5-23 as follows:

$$\sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij}y_{i.}y_{.j} = (5)(23)(9) + (4)(23)(6) + \cdots + (2)(8)(10) = 7236$$
$$SS_N = \frac{\left[\sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij}y_{i.}y_{.j} - y_{..}\left(SS_A + SS_B + \frac{y_{..}^2}{ab}\right)\right]^2}{abSS_ASS_B}$$
$$= \frac{[7236 - (44)(23.33 + 11.60 + 129.07)]^2}{(3)(5)(23.33)(11.60)}$$
$$= \frac{[20.00]^2}{4059.42} = 0.0985$$

and the error sum of squares is, from Equation 5-24,

$$SS_{\text{Error}} = SS_{\text{Residual}} - SS_N$$
$$= 2.00 - 0.0985 = 1.9015$$

The complete analysis of variance is summarized in Table 5-11 on the next page. The test statistic for nonadditivity is $F_0 = 0.0985/0.2716 = 0.36$, so we conclude that there is no evidence of interaction in these data. The main effects of temperature and pressure are significant.

In concluding this section, we note that the two-factor factorial model with one observation per cell (Equation 5-22) looks exactly like the randomized complete block

Table 5-11 Analysis of Variance for Example 5-2

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Temperature	23.33	2	11.67	42.97	0.0001
Pressure	11.60	4	2.90	10.68	0.0042
Nonadditivity	0.0985	1	0.0985	0.36	0.5674
Error	1.9015	7	0.2716		
Total	36.93	14			

model (Equation 4-1). In fact, the Tukey single-degree-of-freedom test for nonadditivity can be directly applied to test for interaction in the randomized block model. However, remember that the **experimental situations** that lead to the randomized block and factorial models are very different. In the factorial model, *all ab* runs have been made in random order, whereas in the randomized block model, randomization occurs only *within the block*. The blocks are a randomization restriction. Hence, the manner in which the experiments are run and the interpretation of the two models are quite different.

5-4 THE GENERAL FACTORIAL DESIGN

The results for the two-factor factorial design may be extended to the general case where there are a levels of factor A, b levels of factor B, c levels of factor C, and so on, arranged in a factorial experiment. In general, there will be $abc \cdots n$ total observations if there are n replicates of the complete experiment. Once again, note that we must have at least two replicates ($n \geq 2$) to determine a sum of squares due to error if all possible interactions are included in the model.

If all factors in the experiment are fixed, we may easily formulate and test hypotheses about the main effects and interactions. For a fixed effects model, test statistics for each main effect and interaction may be constructed by dividing the corresponding mean square for the effect or interaction by the mean square error. All of these F tests will be upper-tail, one-tail tests. The number of degrees of freedom for any main effect is the number of levels of the factor minus one, and the number of degrees of freedom for an interaction is the product of the number of degrees of freedom associated with the individual components of the interaction.

For example, consider the **three-factor analysis of variance model**:

$$y_{ijkl} = \mu + \tau_i + \beta_j + \gamma_k + (\tau\beta)_{ij} + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} + (\tau\beta\gamma)_{ijk} + \epsilon_{ijkl} \quad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, c \\ l = 1, 2, \ldots, n \end{cases} \tag{5-26}$$

Assuming that A, B, and C are fixed, the **analysis of variance table** is shown in Table 5-12. The F tests on main effects and interactions follow directly from the expected mean squares.

Table 5-12 The Analysis of Variance Table for the Three-Factor Fixed Effects Model

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	Expected Mean Square	F_0
A	SS_A	$a-1$	MS_A	$\sigma^2 + \frac{bcn\sum \tau_i^2}{a-1}$	$F_0 = \frac{MS_A}{MS_E}$
B	SS_B	$b-1$	MS_B	$\sigma^2 + \frac{acn\sum \beta_j^2}{b-1}$	$F_0 = \frac{MS_B}{MS_E}$
C	SS_C	$c-1$	MS_C	$\sigma^2 + \frac{abn\sum \gamma_k^2}{c-1}$	$F_0 = \frac{MS_C}{MS_E}$
AB	SS_{AB}	$(a-1)(b-1)$	MS_{AB}	$\sigma^2 + \frac{cn\sum\sum (\tau\beta)_{ij}^2}{(a-1)(b-1)}$	$F_0 = \frac{MS_{AB}}{MS_E}$
AC	SS_{AC}	$(a-1)(c-1)$	MS_{AC}	$\sigma^2 + \frac{bn\sum\sum (\tau\gamma)_{ik}^2}{(a-1)(c-1)}$	$F_0 = \frac{MS_{AC}}{MS_E}$
BC	SS_{BC}	$(b-1)(c-1)$	MS_{BC}	$\sigma^2 + \frac{an\sum\sum (\beta\gamma)_{jk}^2}{(b-1)(c-1)}$	$F_0 = \frac{MS_{BC}}{MS_E}$
ABC	SS_{ABC}	$(a-1)(b-1)(c-1)$	MS_{ABC}	$\sigma^2 + \frac{n\sum\sum\sum (\tau\beta\gamma)_{ijk}^2}{(a-1)(b-1)(c-1)}$	$F_0 = \frac{MS_{ABC}}{MS_E}$
Error	SS_E	$abc(n-1)$	MS_E	σ^2	
Total	SS_T	$abcn-1$			

Usually, the analysis of variance computations would be done using a statistics software package. However, the manual computing formulas for the sums of squares in Table 5-12 are occasionally useful. The total sum of squares is found in the usual way as

$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\sum_{l=1}^{n} y_{ijkl}^2 - \frac{y_{....}^2}{abcn} \tag{5-27}$$

The sums of squares for the main effects are found from the totals for factors $A(y_{i...})$, $B(y_{.j..})$, and $C(y_{..k.})$ as follows:

$$SS_A = \frac{1}{bcn}\sum_{i=1}^{a} y_{i...}^2 - \frac{y_{....}^2}{abcn} \tag{5-28}$$

$$SS_B = \frac{1}{acn}\sum_{j=1}^{b} y_{.j..}^2 - \frac{y_{....}^2}{abcn} \tag{5-29}$$

$$SS_C = \frac{1}{abn}\sum_{k=1}^{c} y_{..k.}^2 - \frac{y_{....}^2}{abcn} \tag{5-30}$$

To compute the two-factor interaction sums of squares, the totals for the $A \times B$, $A \times C$, and $B \times C$ cells are needed. It is frequently helpful to collapse the original data table into three two-way tables to compute these quantities. The sums of squares are found from

$$\begin{aligned} SS_{AB} &= \frac{1}{cn}\sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij..}^2 - \frac{y_{....}^2}{abcn} - SS_A - SS_B \\ &= SS_{\text{Subtotals}(AB)} - SS_A - SS_B \end{aligned} \tag{5-31}$$

$$\begin{aligned} SS_{AC} &= \frac{1}{bn}\sum_{i=1}^{a}\sum_{k=1}^{c} y_{i.k.}^2 - \frac{y_{....}^2}{abcn} - SS_A - SS_C \\ &= SS_{\text{Subtotals}(AC)} - SS_A - SS_C \end{aligned} \tag{5-32}$$

and

$$\begin{aligned} SS_{BC} &= \frac{1}{an}\sum_{j=1}^{b}\sum_{k=1}^{c} y_{.jk.}^2 - \frac{y_{....}^2}{abcn} - SS_B - SS_C \\ &= SS_{\text{Subtotals}(BC)} - SS_B - SS_C \end{aligned} \tag{5-33}$$

Note that the sums of squares for the two-factor subtotals are found from the totals in each two-way table. The three-factor interaction sum of squares is computed from the three-way cell totals $\{y_{ijk.}\}$ as

$$SS_{ABC} = \frac{1}{n}\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c} y_{ijk.}^2 - \frac{y_{....}^2}{abcn} - SS_A - SS_B - SS_C - SS_{AB} - SS_{AC} - SS_{BC} \tag{5-34a}$$

$$= SS_{\text{Subtotals}(ABC)} - SS_A - SS_B - SS_C - SS_{AB} - SS_{AC} - SS_{BC} \tag{5-34b}$$

The error sum of squares may be found by subtracting the sum of squares for each main effect and interaction from the total sum of squares or by

$$SS_E = SS_T - SS_{\text{Subtotals}(ABC)} \tag{5-35}$$

EXAMPLE 5-3

The Soft Drink Bottling Problem

A soft drink bottler is interested in obtaining more uniform fill heights in the bottles produced by his manufacturing process. The filling machine theoretically fills each bottle to the correct target height, but in practice, there is variation around this target, and the bottler would like to understand better the sources of this variability and eventually reduce it.

The process engineer can control three variables during the filling process: the percent carbonation (A), the operating pressure in the filler (B), and the bottles produced per minute or the line speed (C). The pressure and speed are easy to control, but the percent carbonation is more difficult to control during actual manufacturing because it varies with product temperature. However, for purposes of an experiment, the engineer can control carbonation at three levels: 10, 12, and 14 percent. She chooses two levels for pressure (25 and 30 psi) and two levels for line speed (200 and 250 bpm). She decides to run two replicates of a factorial design in these three factors, with all 24 runs taken in random order. The response variable observed is the average deviation from the target fill height observed in a production run of bottles at each set of conditions. The data that resulted from this experiment are shown in Table 5-13. Positive deviations are fill heights above the target, whereas negative deviations are fill heights below the target. The circled numbers in Table 5-13 are the three-way cell totals $y_{ijk\cdot}$.

The total corrected sum of squares is found from Equation 5-27 as

$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\sum_{l=1}^{n} y_{ijkl}^2 - \frac{y_{....}^2}{abcn}$$

$$= 571 - \frac{(75)^2}{24} = 336.625$$

Table 5-13 Fill Height Deviation Data for Example 5-3

	Operating Pressure (B)				
	25 psi		30 psi		
Percent Carbonation (A)	Line Speed (C)		Line Speed (C)		
	200	250	200	250	$y_{i...}$
10	-3, -1 (−4)	-1, 0 (−1)	-1, 0 (−1)	1, 1 (2)	−4
12	0, 1 (1)	2, 1 (3)	2, 3 (5)	6, 5 (11)	20
14	5, 4 (9)	7, 6 (13)	7, 9 (16)	10, 11 (21)	59
$B \times C$ Totals $y_{\cdot jk\cdot}$	6	15	20	34	$75 = y_{....}$
$y_{\cdot j\cdot\cdot}$	21		54		

$A \times B$ Totals $y_{ij\cdot\cdot}$

A \ B	25	30
10	−5	1
12	4	16
14	22	37

$A \times C$ Totals $y_{i\cdot k\cdot}$

A \ C	200	250
10	−5	1
12	6	14
14	25	34

and the sums of squares for the main effects are calculated from Equations 5-28, 5-29, and 5-30 as

$$SS_{\text{Carbonation}} = \frac{1}{bcn}\sum_{i=1}^{a} y_{i...}^2 - \frac{y_{....}^2}{abcn}$$
$$= \frac{1}{8}[(-4)^2 + (20)^2 + (59)^2] - \frac{(75)^2}{24} = 252.750$$
$$SS_{\text{Pressure}} = \frac{1}{acn}\sum_{j=1}^{b} y_{.j..}^2 - \frac{y_{....}^2}{abcn}$$
$$= \frac{1}{12}[(21)^2 + (54)^2] - \frac{(75)^2}{24} = 45.375$$

and

$$SS_{\text{Speed}} = \frac{1}{abn}\sum_{k=1}^{c} y_{..k.}^2 - \frac{y_{....}^2}{abcn}$$
$$= \frac{1}{12}[(26)^2 + (49)^2] - \frac{(75)^2}{24} = 22.042$$

To calculate the sums of squares for the two-factor interactions, we must find the two-way cell totals. For example, to find the carbonation-pressure or AB interaction, we need the totals for the $A \times B$ cells $\{y_{ij..}\}$ shown in Table 5-13. Using Equation 5-31, we find the sums of squares as

$$SS_{AB} = \frac{1}{cn}\sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij..}^2 - \frac{y_{....}^2}{abcn} - SS_A - SS_B$$
$$= \frac{1}{4}[(-5)^2 + (1)^2 + (4)^2 + (16)^2 + (22)^2 + (37)^2] - \frac{(75)^2}{24}$$
$$- 252.750 - 45.375$$
$$= 5.250$$

The carbonation–speed or AC interaction uses the $A \times C$ cell totals $\{y_{i.k.}\}$ shown in Table 5-13 and Equation 5-32:

$$SS_{AC} = \frac{1}{bn}\sum_{i=1}^{a}\sum_{k=1}^{c} y_{i.k.}^2 - \frac{y_{....}^2}{abcn} - SS_A - SS_C$$
$$= \frac{1}{4}[(-5)^2 + (1)^2 + (6)^2 + (14)^2 + (25)^2 + (34)^2] - \frac{(75)^2}{24}$$
$$- 252.750 - 22.042$$
$$= 0.583$$

The pressure–speed or BC interaction is found from the $B \times C$ cell totals $\{y_{.jk.}\}$ shown in Table 5-13 and Equation 5-33:

$$SS_{BC} = \frac{1}{an}\sum_{j=1}^{b}\sum_{k=1}^{c} y_{.jk.}^2 - \frac{y_{....}^2}{abcn} - SS_B - SS_C$$
$$= \frac{1}{6}[(6)^2 + (15)^2 + (20)^2 + (34)^2] - \frac{(75)^2}{24} - 45.375 - 22.042$$
$$= 1.042$$

The three-factor interaction sum of squares is found from the $A \times B \times C$ cell totals $\{y_{ijk.}\}$, which are circled in Table 5-13. From Equation 5-34a, we find

$$\begin{aligned} SS_{ABC} &= \frac{1}{n}\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c} y_{ijk.}^2 - \frac{y_{....}^2}{abcn} - SS_A - SS_B - SS_C - SS_{AB} - SS_{AC} - SS_{BC} \\ &= \frac{1}{2}\left[(-4)^2 + (-1)^2 + (-1)^2 + \cdots + (16)^2 + (21)^2\right] - \frac{(75)^2}{24} \\ &\quad - 252.750 - 45.375 - 22.042 - 5.250 - 0.583 - 1.042 \\ &= 1.083 \end{aligned}$$

Finally, noting that

$$SS_{\text{Subtotals}(ABC)} = \frac{1}{n}\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c} y_{ijk.}^2 - \frac{y_{....}^2}{abcn} = 328.125$$

we have

$$\begin{aligned} SS_E &= SS_T - SS_{\text{Subtotals}(ABC)} \\ &= 336.625 - 328.125 \\ &= 8.500 \end{aligned}$$

The analysis of variance is summarized in Table 5-14. We see that the percentage of carbonation, operating pressure, and line speed significantly affect the fill volume. The carbonation–pressure interaction F ratio has a P-value of 0.0558, indicating some interaction between these factors.

The next step should be an analysis of the residuals from this experiment. We leave this as an exercise for the reader but point out that a normal probability plot of the residuals and the other usual diagnostics do not indicate any major concerns.

To assist in the practical interpretation of this experiment, Figure 5-16 (page 200) presents plots of the three main effects and the AB (carbonation–pressure) interaction. The main effect plots are just graphs of the marginal response averages at the levels of the three factors. Notice that all three variables have *positive* main effects; that is, increasing the variable moves the average deviation from the fill target upward. The interaction between carbonation and pressure is fairly small, as shown by the similar shape of the two curves in Figure 5-16*d*.

Because the company wants the average deviation from the fill target to be close to zero, the engineer decides to recommend the low level of operating pressure (25 psi) and

Table 5-14 Analysis of Variance for Example 5-3

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Percentage of carbonation (A)	252.750	2	126.375	178.412	<0.0001
Operating pressure (B)	45.375	1	45.375	64.059	<0.0001
Line speed (C)	22.042	1	22.042	31.118	0.0001
AB	5.250	2	2.625	3.706	0.0558
AC	0.583	2	0.292	0.412	0.6713
BC	1.042	1	1.042	1.471	0.2485
ABC	1.083	2	0.542	0.765	0.4867
Error	8.500	12	0.708		
Total	336.625	23			

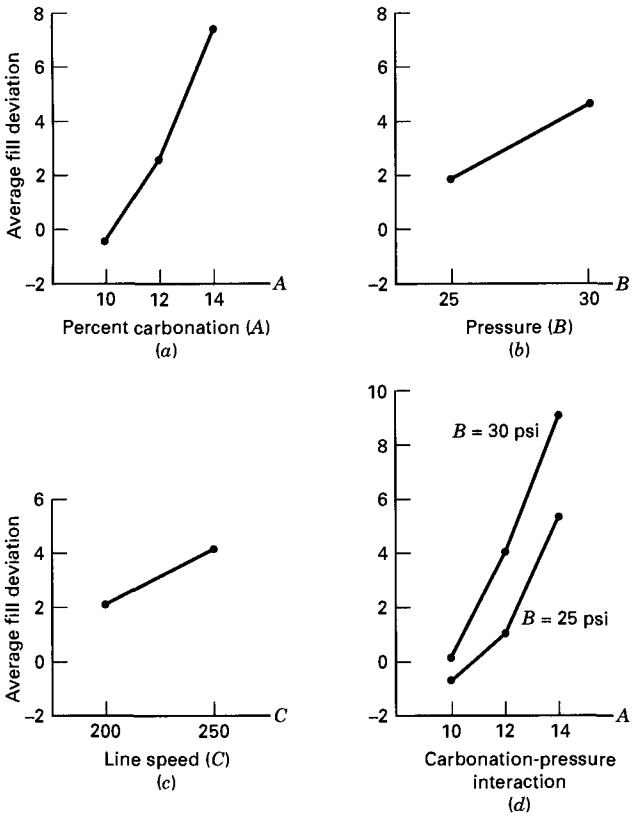


Figure 5-16 Main effects and interaction plots for Example 6-3. (*a*) Percentage of carbonation (*A*). (*b*) Pressure (*B*). (*c*) Line speed (*C*). (*d*) Carbonation-pressure interaction.

the high level of line speed (250 bpm, which will maximize the production rate). Figure 5-17 plots the average observed deviation from the target fill height at the three different carbonation levels for this set of operating conditions. Now the carbonation level cannot presently be perfectly controlled in the manufacturing process, and the normal distribution shown with the solid curve in Figure 5-17 approximates the variability in the car-

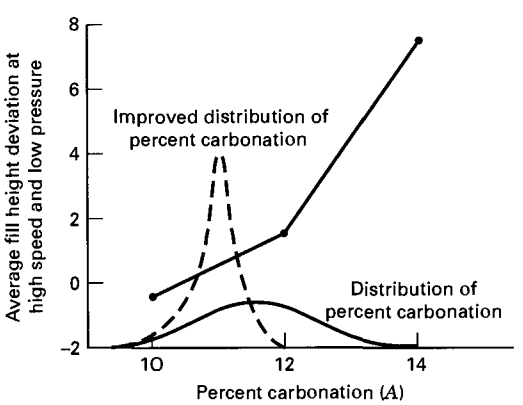


Figure 5-17 Average fill height deviation at high speed and low pressure for different carbonation levels.

bonation levels presently experienced. As the process is impacted by the values of the carbonation level drawn from this distribution, the fill heights will fluctuate considerably. This variability in the fill heights could be reduced if the distribution of the carbonation level values followed the normal distribution shown with the dashed line in Figure 5-17. Reducing the standard deviation of the carbonation level distribution was ultimately achieved by improving temperature control during manufacturing.

We have indicated that if all the factors in a factorial experiment are fixed, test statistic construction is straightforward. The statistic for testing any main effect or interaction is always formed by dividing the mean square for the main effect or interaction by the mean square error. However, if the factorial experiment involves one or more **random factors**, the test statistic construction is not always done this way. We must examine the expected mean squares to determine the correct tests. We defer a complete discussion of experiments with random factors until Chapter 12.

5-5 FITTING RESPONSE CURVES AND SURFACES

We have observed that it can be useful to fit a **response curve** to the levels of a quantitative factor so that the experimenter has an equation that relates the response to the factor. This equation might be used for interpolation, that is, for predicting the response at factor levels between those actually used in the experiment. When at least two factors are quantitative, we can fit a **response surface** for predicting y at various combinations of the design factors. In general, **linear regression methods** are used to fit these models to the experimental data. We illustrated this procedure in Section 3-5.1 for an experiment with a single factor. We now present two examples involving factorial experiments. We will use a computer software package to generate the regression models. For more information about regression analysis, refer to Chapter 10 and the supplemental text material for this chapter.

EXAMPLE 5-4

Consider the experiment described in Example 5-1. The factor temperature is quantitative and material type is qualitative. Furthermore, there are three levels of temperature. Consequently, we can compute a linear and a quadratic temperature effect to study how temperature affects the battery life. Table 5-15 (on the next page) presents condensed output from Design-Expert for this experiment and assumes that temperature is quantitative and material type is qualitative.

The analysis of variance in Table 5-15 shows that the "model" source of variability has been subdivided into several components. The components "A" and "A^2" represent the linear and quadratic effects of temperature, and "B" represents the main effect of the material type factor. Recall that material type is a qualitative factor with three levels. The terms "AB" and "A^2B" are the interactions of the linear and quadratic temperature factor with material type.

The P-values indicate that A^2 and AB are not significant, whereas the A^2B term is significant. Often we think about removing nonsignificant terms or factors from a model but in this case, removing A^2 and AB and retaining A^2B will result in a model that is not

Table 5-15 Design-Expert Output for Example 5-4

Response: Life in hr

ANOVA for Response Surface Reduced Cubic Model

Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Model	59416.22	8	7427.03	11.00	<0.0001	significant
A	*39042.67*	*1*	*39042.67*	*57.82*	*<0.0001*	
B	*10683.72*	*2*	*5341.86*	*7.91*	*0.0020*	
A^2	*76.06*	*1*	*76.06*	*0.11*	*0.7398*	
AB	*2315.08*	*2*	*1157.54*	*1.71*	*0.1991*	
A^2B	*7298.69*	*2*	*3649.35*	*5.40*	*0.0106*	
Residual	18230.75	27	675.21			
Lack of Fit	*0.000*	*0*				
Pure Error	*18230.75*	*27*	*675.21*			
Cor Total	77646.97	35				

Std. Dev.	25.98	R-Squared	0.7652
Mean	105.53	Adj R-Squared	0.6956
C.V.	24.62	Pred R-Squared	0.5826
PRESS	32410.22	Adeq Precision	8.178

Term	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High	VIF
Intercept	107.58	1	7.50	92.19	122.97	
A-Temp	−40.33	1	5.30	−51.22	−29.45	1.00
B[1]	−50.33	1	10.61	−72.10	−28.57	
B[2]	12.17	1	10.61	−9.60	33.93	
A^2	−3.08	1	9.19	−21.93	15.77	1.00
AB[1]	1.71	1	7.50	−13.68	17.10	
AB[2]	−12.79	1	7.50	−28.18	2.60	
$A^2B[1]$	41.96	1	12.99	15.30	68.62	
$A^2B[2]$	−14.04	1	12.99	−40.70	12.62	

Final Equation in Terms of Coded Factors:

$$\begin{aligned}\text{Life} = \\ &+107.58 \\ &-40.33 * A \\ &-50.33 * B[1] \\ &+12.17 * B[2] \\ &-3.08 * A^2 \\ &+1.71 * AB[1] \\ &-12.79 * AB[2] \\ &+41.96 * A^2B[1] \\ &-14.04 * A^2B[2]\end{aligned}$$

Final Equation in Terms of Actual Factors:

Material Type 1

$$\begin{aligned}\text{Life} = \\ &+169.38017 \\ &-2.48860 * \text{Temp} \\ &+0.012851 * \text{Temp}^2\end{aligned}$$

Material Type 2

$$\begin{aligned}\text{Life} = \\ &+159.62397 \\ &-0.17901 * \text{Temp} \\ &+0.41627 * \text{Temp}^2\end{aligned}$$

Material Type 3

$$\begin{aligned}\text{Life} = \\ &+132.76240 \\ &+0.89264 * \text{Temp} \\ &-0.43218 * \text{Temp}^2\end{aligned}$$

hierarchical. The **hierarchy principle** indicates that if a model contains a high-order term (such as A^2B), it should also contain all of the lower-order terms that compose it (in this case A^2 and AB). Hierarchy promotes a type of internal consistency in a model, and many statistical model builders rigorously follow the principal. However, hierarchy is not always a good idea, and many models actually work better as prediction equations without including the nonsignificant terms that promote hierarchy. For more information, see the supplemental text material for this chapter.

The computer output also gives model coefficient estimates and a final prediction equation for battery life in coded factors. In this equation, the levels of temperature are $A = -1, 0, +1$ respectively, when temperature is at the low, middle, and high levels (15, 70, 125°). The variables $B[1]$ and $B[2]$ are coded **indicator variables** that are defined as follows:

	Material Type		
	1	2	3
$B[1]$	1	0	−1
$B[2]$	0	1	−1

There are also prediction equations for battery life in terms of the actual factor levels. Notice that because material type is a qualitative factor there is an equation for predicted life as a function of temperature for each material type. Figure 5-18 shows the response

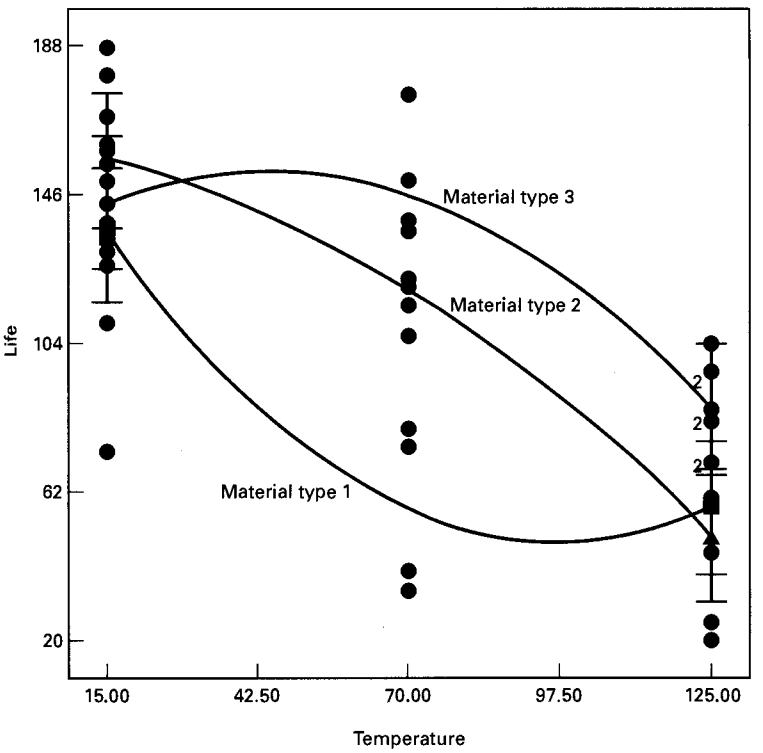


Figure 5-18 Predicted life as a function of temperature for the three material types, Example 5-4.

curves generated by these three prediction equations. Compare them to the two-factor interaction graph for this experiment in Figure 5-9.

If several factors in a factorial experiment are quantitative a **response surface** may be used to model the relationship between y and the design factors. Furthermore, the quantitative factor effects may be represented by single-degree-of-freedom polynomial effects. Similarly, the interactions of quantitative factors can be partitioned into single-degree-of-freedom components of interaction. This is illustrated in the following example.

EXAMPLE 5-5

The effective life of a cutting tool installed in a numerically controlled machine is thought to be affected by the cutting speed and the tool angle. Three speeds and three angles are selected, and a factorial experiment with two replicates is performed. The coded data are shown in Table 5-16. The circled numbers in the cells are the cell totals $\{y_{ij.}\}$.

Condensed Design-Expert output for this example is shown in Table 5-17. The terms A and A^2 are the linear and quadratic effects of tool angle, and B and B^2 are the linear and quadratic effects of speed. The terms AB, A^2B, AB^2, and A^2B^2 represent linear $\times$ linear, quadratic $\times$ linear, linear $\times$ quadratic, and quadratic $\times$ quadratic **components** of the two-factor interaction. Although there are some large P-values, all model terms have been retained to ensure hierarchy. The prediction equation expressed in coded factors uses the levels -1, 0, and $+1$ for A and B to represent the low, middle, and high levels of these factors, respectively.

Figure 5-19 (page 206) presents a **contour plot** of the surface generated by the prediction equation for tool life. Examination of this **response surface** indicates that maximum tool life is achieved at cutting speeds around 150 rpm and tool angles of 25°. The three-dimensional response surface plot in Figure 5-20 (page 206) provides essentially the same information, but it provides a different and sometimes more useful perspective of the tool life response surface. Exploration of response surfaces is a very important aspect of experimental design, which we will discuss in more detail in Chapter 11.

Table 5-16 Data for Tool Life Experiment

Tool Angle (degrees)	Cutting Speed (in/min) 125	150	175	$y_{i..}$
15	-2, -1 (−3)	-3, 0 (−3)	2, 3 (5)	−1
20	0, 2 (2)	1, 3 (4)	4, 6 (10)	16
25	-1, 0 (−1)	5, 6 (11)	0, -1 (−1)	9
$y_{.j.}$	−2	12	14	$24 = y_{...}$

Table 5-17 Design Expert Output for Example 5-5

Response: Life in Hours

ANOVA for Response Surface Reduced Order 4 Model

Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Model	111.00	8	13.87	9.61	0.0013	significant
A	*49.00*	*1*	*49.00*	*33.92*	*0.0003*	
B	*16.00*	*1*	*16.00*	*11.08*	*0.0088*	
A^2	*0.000*	*1*	*0.000*	*0.000*	*1.0000*	
B^2	*1.33*	*1*	*1.33*	*0.92*	*0.3618*	
AB	*8.00*	*1*	*8.00*	*5.54*	*0.0431*	
A^2B	*2.67*	*1*	*2.67*	*1.85*	*0.2073*	
AB^2	*42.67*	*1*	*42.67*	*29.54*	*0.0004*	
A^2B^2	*8.00*	*1*	*8.00*	*5.54*	*0.0431*	
Residual	13.00	9	1.44			
Lack of Fit	*0.000*	*0*				
Pure Error	*13.00*	*9*	*1.44*			
Cor Total	124.00	17				

Std. Dev.	1.20	R-Squared	0.8952
Mean	1.33	Adj R-Squared	0.8020
C.V.	90.14	Pred R-Squared	0.5806
PRESS	52.00	Adeq Precision	8.237

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High	VIF
Intercept	2.00	1	0.85	0.078	3.92	
A-Tool Angle	3.50	1	0.60	2.14	4.86	3.00
B-Speed	2.00	1	0.60	0.64	3.36	3.00
A^2	0.000	1	1.04	−2.35	2.35	3.00
B^2	1.00	1	1.04	−1.35	3.35	3.00
AB	−1.00	1	0.42	−1.96	−0.039	1.00
A^2B	−1.00	1	0.74	−2.66	0.66	3.00
AB^2	−4.00	1	0.74	−5.66	−2.34	3.00
A^2B^2	−3.00	1	1.27	−5.88	−0.12	5.00

Final Equation in Terms of Coded Factors:

$$\begin{aligned}\text{Life} = \\ &+2.00 \\ &+3.50 * A \\ &+2.00 * B \\ &+0.000 * A^2 \\ &+1.00 * B^2 \\ &-1.00 * A * B \\ &-1.00 * A^2 * B \\ &-4.00 * A * B^2 \\ &-3.00 * A^2 * B^2\end{aligned}$$

Final Equation in Terms of Actual Factors:

$$\begin{aligned}\text{Life} = \\ &-1068.00000 \\ &+136.30000 * \text{Tool Angle} \\ &+14.48000 * \text{Speed} \\ &-4.08000 * \text{Tool Angle}^2 \\ &-0.049600 * \text{Speed}^2 \\ &-1.86400 * \text{Tool Angle} * \text{Speed} \\ &+0.056000 * \text{Tool Angle}^2 * \text{Speed} \\ &+6.40000\text{E}-003 * \text{Tool Angle} * \text{Speed}^2 \\ &-1.92000\text{E}-004 * \text{Tool Angle}^2 * \text{Speed}^2\end{aligned}$$

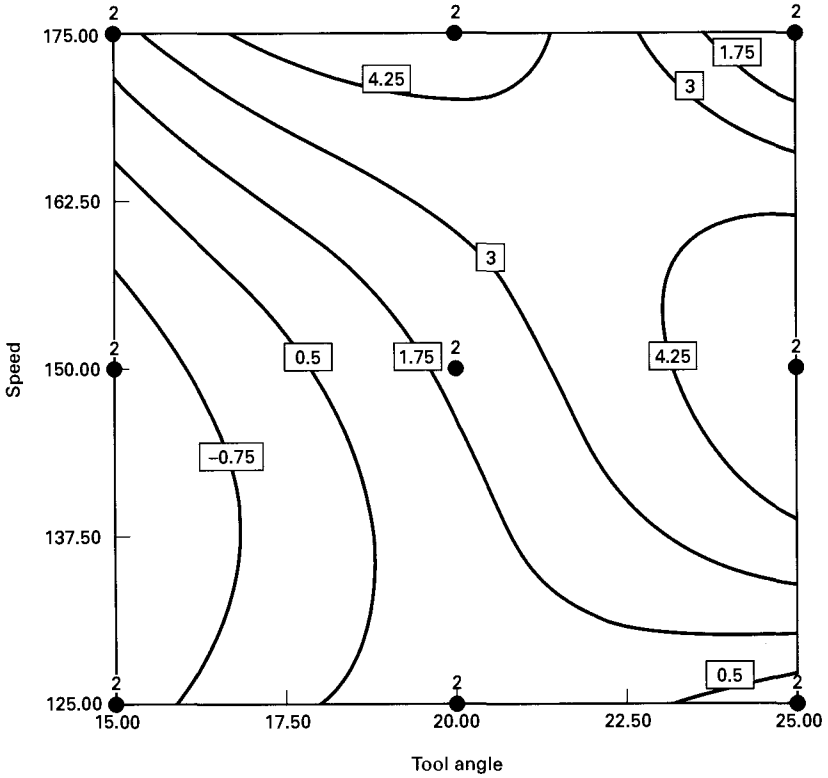


Figure 5-19 Two-dimensional contour plot of the tool life response surface for Example 5-5.

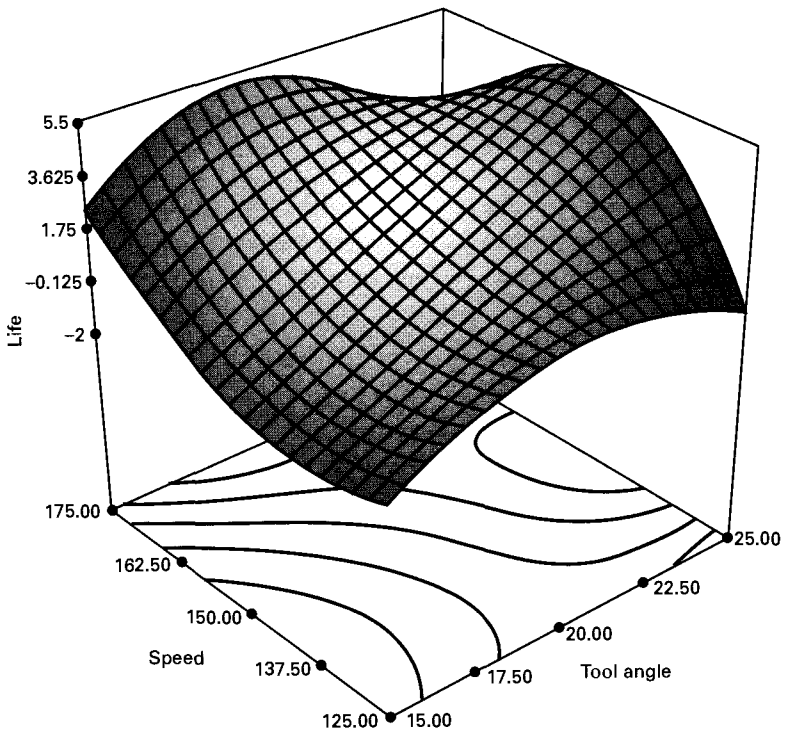


Figure 5-20 Three-dimensional tool life response surface for Example 5-5.

5-6 BLOCKING IN A FACTORIAL DESIGN

We have discussed factorial designs in the context of a **completely randomized** experiment. Sometimes, it is not feasible or practical to completely randomize all of the runs in a factorial. For example, the presence of a nuisance factor may require that the experiment be run in **blocks**. We discussed the basic concepts of blocking in the context of a single-factor experiment in Chapter 4. We now show how blocking can be incorporated in a factorial. Some other aspects of blocking in factorial designs are presented in Chapters 7, 8, 9, and 13.

Consider a factorial experiment with two factors (A and B) and n replicates. The linear statistical model for this design is

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases} \tag{5-36}$$

where τ_i, β_j, and $(\tau\beta)_{ij}$ represent the effects of factors A, B, and the AB interaction, respectively. Now suppose that to run this experiment a particular raw material is required. This raw material is available in batches that are not large enough to allow *all abn* treatment combinations to be run from the *same* batch. However, if a batch contains enough material for ab observations, then an alternative design is to run each of the n replicates using a separate batch of raw material. Consequently, the batches of raw material represent a randomization restriction or a **block**, and a single replicate of a complete factorial experiment is run within each block. The effects model for this new design is

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \delta_k + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases} \tag{5-37}$$

where δ_k is the effect of the kth block. Of course, within a block the order in which the treatment combinations are run is completely randomized.

The model (Equation 5-37) assumes that interaction between blocks and treatments is negligible. This was assumed previously in the analysis of randomized block designs. If these interactions do exist, they cannot be separated from the error component. In fact, the error term in this model really consists of the $(\tau\delta)_{ik}$, $(\beta\delta)_{jk}$, and $(\tau\beta\delta)_{ijk}$ interactions. The analysis of variance is outlined in Table 5-18 on page 208. The layout closely resembles that of a factorial design, with the error sum of squares reduced by the sum of squares for blocks. Computationally, we find the sum of squares for blocks as the sum of squares between the n block totals $\{y_{..k}\}$.

In the previous example, the randomization was restricted to within a batch of raw material. In practice, a variety of phenomena may cause randomization restrictions, such as time, operators, and so on. For example, if we could not run the entire factorial experiment on one day, then the experimenter could run a complete replicate on day 1, a second replicate on day 2, and so on. Consequently, each day would be a block.

EXAMPLE 5-6

An engineer is studying methods for improving the ability to detect targets on a radar scope. Two factors she considers to be important are the amount of background noise, or "ground clutter," on the scope and the type of filter placed over the screen. An

Table 5-18 Analysis of Variance for a Two-Factor Factorial in a Randomized Complete Block

Source of Variation	Sum of Squares	Degrees of Freedom	Expected Mean Square	F_0
Blocks	$\frac{1}{ab}\sum_k y_{..k}^2 - \frac{y_{...}^2}{abn}$	$n-1$	$\sigma^2 + ab\sigma_\delta^2$	
A	$\frac{1}{bn}\sum_i y_{i..}^2 - \frac{y_{...}^2}{abn}$	$a-1$	$\sigma^2 + \frac{bn\sum \tau_i^2}{a-1}$	$\frac{MS_A}{MS_E}$
B	$\frac{1}{an}\sum_j y_{.j.}^2 - \frac{y_{...}^2}{abn}$	$b-1$	$\sigma^2 + \frac{an\sum \beta_j^2}{b-1}$	$\frac{MS_B}{MS_E}$
AB	$\frac{1}{n}\sum_i\sum_j y_{ij.}^2 - \frac{y_{...}^2}{abn} - SS_A - SS_B$	$(a-1)(b-1)$	$\sigma^2 + \frac{n\sum\sum (\tau\beta)_{ij}^2}{(a-1)(b-1)}$	$\frac{MS_{AB}}{MS_E}$
Error	Subtraction	$(ab-1)(n-1)$	σ^2	
Total	$\sum_i\sum_j\sum_k y_{ijk}^2 - \frac{y_{...}^2}{abn}$	$abn-1$		

experiment is designed using three levels of ground clutter and two filter types. We will consider these as fixed type factors. The experiment is performed by randomly selecting a treatment combination (ground clutter level and filter type) and then introducing a signal representing the target into the scope. The intensity of this target is increased until the operator observes it. The intensity level at detection is then measured as the response variable. Because of operator availability, it is convenient to select an operator and keep him or her at the scope until all the necessary runs have been made. Furthermore, operators differ in their skill and ability to use the scope. Consequently, it seems logical to use the operators as blocks. Four operators are randomly selected. Once an operator is chosen, the order in which the six treatment combinations are run is randomly determined. Thus, we have a 3×2 factorial experiment run in a randomized complete block. The data are shown in Table 5-19.

The linear model for this experiment is

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \delta_k + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, 3 \\ j = 1, 2 \\ k = 1, 2, 3, 4 \end{cases}$$

where τ_i represents the ground clutter effect, β_j represents the filter type effect, $(\tau\beta)_{ij}$ is the interaction, δ_k is the block effect, and ϵ_{ijk} is the NID(0, σ^2) error component. The sums of squares for ground clutter, filter type, and their interaction are computed in the

Table 5-19 Intensity Level at Target Detection

Operators (blocks)	1		2		3		4	
Filter Type	1	2	1	2	1	2	1	2
Ground clutter								
Low	90	86	96	84	100	92	92	81
Medium	102	87	106	90	105	97	96	80
High	114	93	112	91	108	95	98	83

Table 5-20 Analysis of Variance for Example 5-6

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Ground clutter (G)	335.58	2	167.79	15.13	0.0003
Filter type (F)	1066.67	1	1066.67	96.19	<0.0001
GF	77.08	2	38.54	3.48	0.0573
Blocks	402.17	3	134.06		
Error	166.33	15	11.09		
Total	2047.83	23			

usual manner. The sum of squares due to blocks is found from the operator totals $\{y_{..k}\}$ as follows:

$$\begin{aligned} SS_{\text{Blocks}} &= \frac{1}{ab}\sum_{k=1}^{n} y_{..k}^2 - \frac{y_{...}^2}{abn} \\ &= \frac{1}{(3)(2)}[(572)^2 + (579)^2 + (597)^2 + (530)^2] - \frac{(2278)^2}{(3)(2)(4)} \\ &= 402.17 \end{aligned}$$

The complete analysis of variance for this experiment is summarized in Table 5-20. The presentation in Table 5-20 indicates that all effects are tested by dividing their mean squares by the mean square error. Both ground clutter level and filter type are significant at the 1 percent level, whereas their interaction is significant only at the 10 percent level. Thus, we conclude that both ground clutter level and the type of scope filter used affect the operator's ability to detect the target, and there is some evidence of mild interaction between these factors.

In the case of two randomization restrictions, each with p levels, if the number of treatment combinations in a k-factor factorial design exactly equals the number of restriction levels, that is, if $p = ab \ldots m$, then the factorial design may be run in a $p \times p$ Latin square. For example, consider a modification of the radar target detection experiment of Example 5-6. The factors in this experiment are filter type (two levels) and ground clutter (three levels), and operators are considered as blocks. Suppose now that because of the setup time required, only six runs can be made per day. Thus, days become a second randomization restriction, resulting in the 6×6 Latin square design, as shown in Table 5-21 on the next page. In this table we have used the lowercase letters f_i and g_j to represent the ith and jth levels of filter type and ground clutter, respectively. That is, f_1g_2 represents filter type 1 and medium ground clutter. Note that now six operators are required, rather than four as in the original experiment, so the number of treatment combinations in the 3×2 factorial design exactly equals the number of restriction levels. Furthermore, in this design, each operator would be used only once on each day. The Latin letters A, B, C, D, E, and F represent the $3 \times 2 = 6$ factorial treatment combinations as follows: $A = f_1g_1$, $B = f_1g_2$, $C = f_1g_3$, $D = f_2g_1$, $E = f_2g_2$, and $F = f_2g_3$.

The five degrees of freedom between the six Latin letters correspond to the main effects of filter type (one degree of freedom), ground clutter (two degrees of freedom),

Table 5-21 Radar Detection Experiment Run in a 6 × 6 Latin Square

	Operator					
Day	1	2	3	4	5	6
1	$A(f_1g_1 = 90)$	$B(f_1g_2 = 106)$	$C(f_1g_3 = 108)$	$D(f_2g_1 = 81)$	$F(f_2g_3 = 90)$	$E(f_2g_2 = 88)$
2	$C(f_1g_3 = 114)$	$A(f_1g_1 = 96)$	$B(f_1g_2 = 105)$	$F(f_2g_3 = 83)$	$E(f_2g_2 = 86)$	$D(f_2g_1 = 84)$
3	$B(f_1g_2 = 102)$	$E(f_2g_2 = 90)$	$F(f_2g_3 = 95)$	$A(f_1g_1 = 92)$	$D(f_2g_1 = 85)$	$C(f_1g_3 = 104)$
4	$E(f_2g_2 = 87)$	$D(f_2g_1 = 84)$	$A(f_1g_1 = 100)$	$B(f_1g_2 = 96)$	$C(f_1g_3 = 110)$	$F(f_2g_3 = 91)$
5	$F(f_2g_3 = 93)$	$C(f_1g_3 = 112)$	$D(f_2g_1 = 92)$	$E(f_2g_2 = 80)$	$A(f_1g_1 = 90)$	$B(f_1g_2 = 98)$
6	$D(f_2g_1 = 86)$	$F(f_2g_3 = 91)$	$E(f_2g_2 = 97)$	$C(f_1g_3 = 98)$	$B(f_1g_2 = 100)$	$A(f_1g_1 = 92)$

and their interaction (two degrees of freedom). The linear statistical model for this design is

$$y_{ijkl} = \mu + \alpha_i + \tau_j + \beta_k + (\tau\beta)_{jk} + \theta_l + \epsilon_{ijkl} \qquad \begin{cases} i = 1, 2, \ldots, 6 \\ j = 1, 2, 3 \\ k = 1, 2 \\ l = 1, 2, \ldots, 6 \end{cases} \tag{5-38}$$

where τ_j and β_k are effects of ground clutter and filter type, respectively, and α_i and θ_l represent the randomization restrictions of days and operators, respectively. To compute the sums of squares, the following two-way table of treatment totals is helpful:

Ground Clutter	Filter Type 1	Filter Type 2	$y_{.j.}$
Low	560	512	1072
Medium	607	528	1135
High	646	543	1189
$y_{..k.}$	1813	1583	$3396 = y_{....}$

Furthermore, the row and column totals are

Rows ($y_{.jkl}$):	563	568	568	568	565	564
Columns ($y_{ijk.}$):	572	579	597	530	561	557

The analysis of variance is summarized in Table 5-22. We have added a column to this table indicating how the number of degrees of freedom for each sum of squares is determined.

Table 5-22 Analysis of Variance for the Radar Detection Experiment Run as a 3 × 2 Factorial in a Latin Square

Source of Variation	Sum of Squares	Degrees of Freedom	General Formula for Degrees of Freedom	Mean Square	F_0	P-Value
Ground clutter, G	571.50	2	$a - 1$	285.75	28.86	<0.0001
Filter type, F	1469.44	1	$b - 1$	1469.44	148.43	<0.0001
GF	126.73	2	$(a - 1)(b - 1)$	63.37	6.40	0.0071
Days (rows)	4.33	5	$ab - 1$	0.87		
Operators (columns)	428.00	5	$ab - 1$	85.60		
Error	198.00	20	$(ab - 1)(ab - 2)$	9.90		
Total	2798.00	35	$(ab)^2 - 1$			

5-7 PROBLEMS

5-1. The yield of a chemical process is being studied. The two most important variables are thought to be the pressure and the temperature. Three levels of each factor are selected, and a factorial experiment with two replicates is performed. The yield data follow:

	Pressure (psig)		
Temperature (°C)	200	215	230
150	90.4	90.7	90.2
	90.2	90.6	90.4
160	90.1	90.5	89.9
	90.3	90.6	90.1
170	90.5	90.8	90.4
	90.7	90.9	90.1

(a) Analyze the data and draw conclusions. Use $\alpha = 0.05$.
(b) Prepare appropriate residual plots and comment on the model's adequacy.
(c) Under what conditions would you operate this process?

5-2. An engineer suspects that the surface finish of a metal part is influenced by the feed rate and the depth of cut. He selects three feed rates and four depths of cut. He then conducts a factorial experiment and obtains the following data:

	Depth of Cut (in)			
Feed Rate (in/min)	0.15	0.18	0.20	0.25
	74	79	82	99
0.20	64	68	88	104
	60	73	92	96
	92	98	99	104
0.25	86	104	108	110
	88	88	95	99
	99	104	108	114
0.30	98	99	110	111
	102	95	99	107

(a) Analyze the data and draw conclusions. Use $\alpha = 0.05$.
(b) Prepare appropriate residual plots and comment on the model's adequacy.
(c) Obtain point estimates of the mean surface finish at each feed rate.
(d) Find the P-values for the tests in part (a).

5-3. For the data in Problem 5-2, compute a 95 percent confidence interval estimate of the mean difference in response for feed rates of 0.20 and 0.25 in/min.

5-4. An article in *Industrial Quality Control* (1956, pp. 5–8) describes an experiment to investigate the effect of the type of glass and the type of phosphor on the brightness of a television tube. The response variable is the current necessary (in microamps) to obtain a specified brightness level. The data are as follows:

Glass Type	Phosphor Type 1	2	3
1	280	300	290
	290	310	285
	285	295	290
2	230	260	220
	235	240	225
	240	235	230

(a) Is there any indication that either factor influences brightness? Use $\alpha = 0.05$.
(b) Do the two factors interact? Use $\alpha = 0.05$.
(c) Analyze the residuals from this experiment.

5-5. Johnson and Leone (*Statistics and Experimental Design in Engineering and the Physical Sciences*, Wiley, 1977) describe an experiment to investigate warping of copper plates. The two factors studied were the temperature and the copper content of the plates. The response variable was a measure of the amount of warping. The data were as follows:

Temperature (°C)	Copper Content (%) 40	60	80	100
50	17, 20	16, 21	24, 22	28, 27
75	12, 9	18, 13	17, 12	27, 31
100	16, 12	18, 21	25, 23	30, 23
125	21, 17	23, 21	23, 22	29, 31

(a) Is there any indication that either factor affects the amount of warping? Is there any interaction between the factors? Use $\alpha = 0.05$.
(b) Analyze the residuals from this experiment.
(c) Plot the average warping at each level of copper content and compare them to an appropriately scaled t distribution. Describe the differences in the effects of the different levels of copper content on warping. If low warping is desirable, what level of copper content would you specify?
(d) Suppose that temperature cannot be easily controlled in the environment in which the copper plates are to be used. Does this change your answer for part (c)?

5-6. The factors that influence the breaking strength of a synthetic fiber are being studied. Four production machines and three operators are chosen and a factorial experiment is run using fiber from the same production batch. The results are as follows:

Operator	Machine 1	2	3	4
1	109	110	108	110
	110	115	109	108
2	110	110	111	114
	112	111	109	112
3	116	112	114	120
	114	115	119	117

(a) Analyze the data and draw conclusions. Use $\alpha = 0.05$.
(b) Prepare appropriate residual plots and comment on the model's adequacy.

5-7. A mechanical engineer is studying the thrust force developed by a drill press. He suspects that the drilling speed and the feed rate of the material are the most important factors. He selects four feed rates and uses a high and low drill speed chosen to represent the extreme operating conditions. He obtains the following results. Analyze the data and draw conclusions. Use $\alpha = 0.05$.

	Feed Rate			
Drill Speed	0.015	0.030	0.045	0.060
125	2.70	2.45	2.60	2.75
	2.78	2.49	2.72	2.86
200	2.83	2.85	2.86	2.94
	2.86	2.80	2.87	2.88

5-8. An experiment is conducted to study the influence of operating temperature and three types of face-plate glass in the light output of an oscilloscope tube. The following data are collected:

	Temperature		
Glass Type	100	125	150
	580	1090	1392
1	568	1087	1380
	570	1085	1386
	550	1070	1328
2	530	1035	1312
	579	1000	1299
	546	1045	867
3	575	1053	904
	599	1066	889

(a) Use $\alpha = 0.05$ in the analysis. Is there a significant interaction effect? Does glass type or temperature affect the response? What conclusions can you draw?
(b) Fit an appropriate model relating light output to glass type and temperature.
(c) Analyze the residuals from this experiment. Comment on the adequacy of the models you have considered.

5-9. Consider the experiment in Problem 5-1. Fit an appropriate model to the response data. Use this model to provide guidance concerning operating conditions for the process.

5-10. Use Tukey's test to determine which levels of the pressure factor are significantly different for the data in Problem 5-1.

5-11. An experiment was conducted to determine if either firing temperature or furnace position affects the baked density of a carbon anode. The data are shown below:

	Temperature (°C)		
Position	800	825	850
1	570	1063	565
	565	1080	510
	583	1043	590
2	528	988	526
	547	1026	538
	521	1004	532

Suppose we assume that no interaction exists. Write down the statistical model. Conduct the analysis of variance and test hypotheses on the main effects. What conclusions can be drawn? Comment on the model's adequacy.

5-12. Derive the expected mean squares for a two-factor analysis of variance with one observation per cell, assuming that both factors are fixed.

5-13. Consider the following data from a two-factor factorial experiment. Analyze the data and draw conclusions. Perform a test for nonadditivity. Use $\alpha = 0.05$.

	Column Factor			
Row Factor	1	2	3	4
1	36	39	36	32
2	18	20	22	20
3	30	37	33	34

5-14. The shear strength of an adhesive is thought to be affected by the application pressure and temperature. A factorial experiment is performed in which both factors are assumed to be fixed. Analyze the data and draw conclusions. Perform a test for nonadditivity.

Pressure	Temperature (°F)		
(lb/in^2)	250	260	270
120	9.60	11.28	9.00
130	9.69	10.10	9.57
140	8.43	11.01	9.03
150	9.98	10.44	9.80

5-15. Consider the three-factor model

$$y_{ijk} = \mu + \tau_i + \beta_j + \gamma_k + (\tau\beta)_{ij} + (\beta\gamma)_{jk} + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, c \end{cases}$$

Notice that there is only one replicate. Assuming all the factors are fixed, write down the analysis of variance table, including the expected mean squares. What would you use as the "experimental error" to test hypotheses?

5-16. The percentage of hardwood concentration in raw pulp, the vat pressure, and the cooking time of the pulp are being investigated for their effects on the strength of paper. Three levels of hardwood concentration, three levels of pressure, and two cooking times are selected. A factorial experiment with two replicates is conducted, and the following data are obtained:

Percentage of Hardwood Concentration	Cooking Time 3.0 Hours			Cooking Time 4.0 Hours		
	Pressure			Pressure		
	400	500	650	400	500	650
2	196.6	197.7	199.8	198.4	199.6	200.6
	196.0	196.0	199.4	198.6	200.4	200.9
4	198.5	196.0	198.4	197.5	198.7	199.6
	197.2	196.9	197.6	198.1	198.0	199.0
8	197.5	195.6	197.4	197.6	197.0	198.5
	196.6	196.2	198.1	198.4	197.8	199.8

(a) Analyze the data and draw conclusions. Use $\alpha = 0.05$.
(b) Prepare appropriate residual plots and comment on the model's adequacy.
(c) Under what set of conditions would you operate this process? Why?

5-17. The quality control department of a fabric finishing plant is studying the effect of several factors on the dyeing of cotton–synthetic cloth used to manufacture men's shirts. Three operators, three cycle times, and two temperatures were selected, and three small specimens of cloth were dyed under each set of conditions. The finished cloth was compared to a standard, and a numerical score was assigned. The results follow. Analyze the data and draw conclusions. Comment on the model's adequacy.

	Temperature					
	300°			350°		
	Operator			Operator		
Cycle Time	1	2	3	1	2	3
	23	27	31	24	38	34
40	24	28	32	23	36	36
	25	26	29	28	35	39
	36	34	33	37	34	34
50	35	38	34	39	38	36
	36	39	35	35	36	31
	28	35	26	26	36	28
60	24	35	27	29	37	26
	27	34	25	25	34	24

5-18. In Problem 5-1, suppose that we wish to reject the null hypothesis with a high probability if the difference in the true mean yield at any two pressures is as great as 0.5. If a reasonable prior estimate of the standard deviation of yield is 0.1, how many replicates should be run?

5-19. The yield of a chemical process is being studied. The two factors of interest are temperature and pressure. Three levels of each factor are selected; however, only nine runs can

be made in one day. The experimenter runs a complete replicate of the design on each day. The data are shown in the following table. Analyze the data, assuming that the days are blocks.

	Day 1 Pressure			Day 2 Pressure		
Temperature	250	260	270	250	260	270
Low	86.3	84.0	85.8	86.1	85.2	87.3
Medium	88.5	87.3	89.0	89.4	89.9	90.3
High	89.1	90.2	91.3	91.7	93.2	93.7

5-20. Consider the data in Problem 5-5. Analyze the data, assuming that replicates are blocks.

5-21. Consider the data in Problem 5-6. Analyze the data, assuming that replicates are blocks.

5-22. An article in the *Journal of Testing and Evaluation* (Vol. 16, no. 2, pp. 508–515) investigated the effects of cyclic loading and environmental conditions on fatigue crack growth at a constant 22 MPa stress for a particular material. The data from this experiment are shown below (the response is crack growth rate):

	Environment		
Frequency	Air	H_2O	Salt H_2O
10	2.29	2.06	1.90
	2.47	2.05	1.93
	2.48	2.23	1.75
	2.12	2.03	2.06
1	2.65	3.20	3.10
	2.68	3.18	3.24
	2.06	3.96	3.98
	2.38	3.64	3.24
0.1	2.24	11.00	9.96
	2.71	11.00	10.01
	2.81	9.06	9.36
	2.08	11.30	10.40

(a) Analyze the data from this experiment (use $\alpha = 0.05$).

(b) Analyze the residuals.

(c) Repeat the analyses from parts (a) and (b) using $\ln(y)$ as the response. Comment on the results.

5-23. An article in the *IEEE Transactions on Electron Devices* (Nov. 1986, pp. 1754) describes a study on polysilicon doping. The experiment shown below is a variation of their study. The response variable is base current.

Polysilicon Doping (ions)	Anneal Temperature (°C)		
	900	950	1000
1×10^{20}	4.60	10.15	11.01
	4.40	10.20	10.58
2×10^{20}	3.20	9.38	10.81
	3.50	10.02	10.60

(a) Is there evidence (with $\alpha = 0.05$) indicating that either polysilicon doping level or anneal temperature affect base current?
(b) Prepare graphical displays to assist in interpretation of this experiment.
(c) Analyze the residuals and comment on model adequacy.
(d) Is the model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \epsilon$$

supported by this experiment (x_1 = doping level, x_2 = temperature)? Estimate the parameters in this model and plot the response surface.

6 The 2^k Factorial Design

6-1 INTRODUCTION

Factorial designs are widely used in experiments involving several factors where it is necessary to study the joint effect of the factors on a response. Chapter 5 presented general methods for the analysis of factorial designs. However, there are several special cases of the general factorial design that are important because they are widely used in research work and also because they form the basis of other designs of considerable practical value.

The most important of these special cases is that of k factors, each at only two levels. These levels may be quantitative, such as two values of temperature, pressure, or time; or they may be qualitative, such as two machines, two operators, the "high" and "low" levels of a factor, or perhaps the presence and absence of a factor. A complete replicate of such a design requires $2 \times 2 \times \cdots \times 2 = 2^k$ observations and is called a **2^k factorial design**.

This chapter focuses on this extremely important class of designs. Throughout this chapter we assume that (1) the factors are fixed, (2) the designs are completely randomized, and (3) the usual normality assumptions are satisfied.

The 2^k design is particularly useful in the early stages of experimental work, when there are likely to be many factors to be investigated. It provides the smallest number of runs with which k factors can be studied in a complete factorial design. Consequently, these designs are widely used in **factor screening experiments**.

Because there are only two levels for each factor, we assume that the response is approximately linear over the range of the factor levels chosen. In many factor screening experiments, when we are just starting to study the process or system, this is often a reasonable assumption. In Section 6-6, we will present a simple method for checking this assumption, and discuss what action to take if it is violated.

6-2 THE 2^2 DESIGN

The first design in the 2^k series is one with only two factors, say A and B, each run at two levels. This design is called a **2^2 factorial design**. The levels of the factors may be arbitrarily called "low" and "high." As an example, consider an investigation into the effect of the concentration of the reactant and the amount of the catalyst on the conversion (yield) in a chemical process. Let the reactant concentration be factor A, and let the two levels of interest be 15 and 25 percent. The catalyst is factor B, with the high level denoting the use of 2 pounds of the catalyst and the low level denoting the use of only 1 pound. The experiment is replicated three times, and the data are as follows:

Factor		Treatment	Replicate			
A	B	Combination	I	II	III	Total
−	−	A low, B low	28	25	27	80
+	−	A high, B low	36	32	32	100
−	+	A low, B high	18	19	23	60
+	+	A high, B high	31	30	29	90

The treatment combinations in this design are shown graphically in Figure 6-1. By convention, we denote the effect of a factor by a capital Latin letter. Thus "A" refers to the effect of factor A, "B" refers to the effect of factor B, and "AB" refers to the AB interaction. In the 2^2 design the low and high levels of A and B are denoted by "−" and "+," respectively, on the A and B axes. Thus, − on the A axis represents the low level of concentration (15%), whereas + represents the high level (25%), and − on the B axis represents the low level of catalyst, whereas + denotes the high level.

The four treatment combinations in the design are usually represented by lowercase letters, as shown in Figure 6-1. We see from the figure that the high level of any factor in the treatment combination is denoted by the corresponding lowercase letter and that the low level of a factor in the treatment combination is denoted by the absence of the

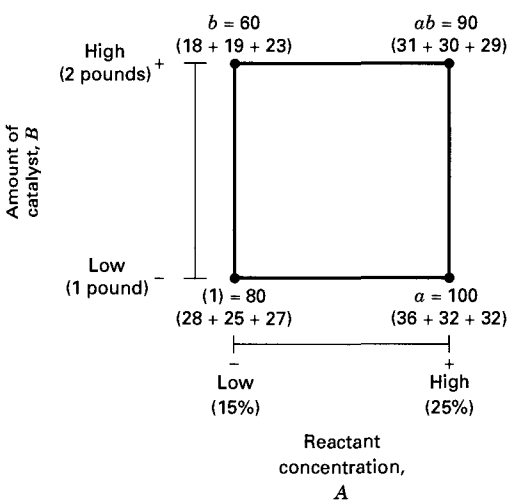


Figure 6-1 Treatment combinations in the 2^2 design.

corresponding letter. Thus, a represents the treatment combination of A at the high level and B at the low level, b represents A at the low level and B at the high level, and ab represents both factors at the high level. By convention, (1) is used to denote both factors at the low level. This notation is used throughout the 2^k series.

In a two-level factorial design, we may define the average effect of a factor as the change in response produced by a change in the level of that factor averaged over the levels of the other factor. Also, the symbols (1), a, b, and ab now represent the *total* of all n replicates taken at the treatment combination, as illustrated in Figure 6-1. Now the effect of A at the low level of B is $[a - (1)]/n$ and the effect of A at the high level of B is $[ab - b]/n$. Averaging these two quantities yields the **main effect** of A:

$$\begin{aligned} A &= \frac{1}{2n}\{[ab - b] + [a - (1)]\} \\ &= \frac{1}{2n}[ab + a - b - (1)] \end{aligned} \tag{6-1}$$

The average main effect of B is found from the effect of B at the low level of A (i.e., $[b - (1)]/n$) and at the high level of A (i.e., $[ab - a]/n$) as

$$\begin{aligned} B &= \frac{1}{2n}\{[ab - a] + [b - (1)]\} \\ &= \frac{1}{2n}[ab + b - a - (1)] \end{aligned} \tag{6-2}$$

We define the **interaction effect** AB as the average difference between the effect of A at the high level of B and the effect of A at the low level of B. Thus,

$$\begin{aligned} AB &= \frac{1}{2n}\{[ab - b] - [a - (1)]\} \\ &= \frac{1}{2n}[ab + (1) - a - b] \end{aligned} \tag{6-3}$$

Alternatively, we may define AB as the average difference between the effect of B at the high level of A and the effect of B at the low level of A. This will also lead to Equation 6-3.

The formulas for the effects of A, B, and AB may be derived by another method. The effect of A can be found as the difference in the average response of the two treatment combinations on the right-hand side of the square in Figure 6-1 (call this average $\bar{y}_{A^+}$, because it is the average response at the treatment combinations where A is at the high level) and the two treatment combinations on the left-hand side (or $\bar{y}_{A^-}$). That is,

$$\begin{aligned} A &= \bar{y}_{A^+} - \bar{y}_{A^-} \\ &= \frac{ab + a}{2n} - \frac{b + (1)}{2n} \\ &= \frac{1}{2n}[ab + a - b - (1)] \end{aligned}$$

This is exactly the same result as in Equation 6-1. The effect of B, Equation 6-2, is found as the difference between the average of the two treatment combinations on the

top of the square ($\bar{y}_{B+}$) and the average of the two treatment combinations on the bottom ($\bar{y}_{B-}$), or

$$\begin{aligned} B &= \bar{y}_{B+} - \bar{y}_{B-} \\ &= \frac{ab + b}{2n} - \frac{a + (1)}{2n} \\ &= \frac{1}{2n}[ab + b - a - (1)] \end{aligned}$$

Finally, the interaction effect AB is the average of the right-to-left diagonal treatment combinations in the square [ab and (1)] minus the average of the left-to-right diagonal treatment combinations (a and b), or

$$\begin{aligned} AB &= \frac{ab + (1)}{2n} - \frac{a + b}{2n} \\ &= \frac{1}{2n}[ab + (1) - a - b] \end{aligned}$$

which is identical to Equation 6-3.

Using the experiment in Figure 6-1, we may estimate the average effects as

$$A = \frac{1}{2(3)}(90 + 100 - 60 - 80) = 8.33$$

$$B = \frac{1}{2(3)}(90 + 60 - 100 - 80) = -5.00$$

$$AB = \frac{1}{2(3)}(90 + 80 - 100 - 60) = 1.67$$

The effect of A (reactant concentration) is positive; this suggests that increasing A from the low level (15%) to the high level (25%) will increase the yield. The effect of B (catalyst) is negative; this suggests that increasing the amount of catalyst added to the process will decrease the yield. The interaction effect appears to be small relative to the two main effects.

In many experiments involving 2^k designs, we will examine the **magnitude** and **direction** of the factor effects to determine which variables are likely to be important. The analysis of variance can generally be used to confirm this interpretation. There are several excellent statistics software packages that are useful for setting up and analyzing 2^k designs. There are also special time-saving methods for performing the calculations manually.

Consider the sums of squares for A, B, and AB. Note from Equation 6-1 that a **contrast** is used in estimating A, namely

$$\text{Contrast}_A = ab + a - b - (1) \tag{6-4}$$

We usually call this contrast the **total effect** of A. From Equations 6-2 and 6-3, we see that contrasts are also used to estimate B and AB. Furthermore, these three contrasts are **orthogonal**. The sum of squares for any contrast can be computed from Equation 3-29, which states that the contrast sum of squares is equal to the contrast squared divided by

the number of observations in each total in the contrast times the sum of the squares of the contrast coefficients. Consequently, we have

$$SS_A = \frac{[ab + a - b - (1)]^2}{4n} \tag{6-5}$$

$$SS_B = \frac{[ab + b - a - (1)]^2}{4n} \tag{6-6}$$

and

$$SS_{AB} = \frac{[ab + (1) - a - b]^2}{4n} \tag{6-7}$$

as the sums of squares for A, B, and AB.

Using the experiment in Figure 6-1, we may find the sums of squares from Equations 6-5, 6-6, and 6-7 as

$$SS_A = \frac{(50)^2}{4(3)} = 208.33$$

$$SS_B = \frac{(-30)^2}{4(3)} = 75.00 \tag{6-8}$$

and

$$SS_{AB} = \frac{(10)^2}{4(3)} = 8.33$$

The total sum of squares is found in the usual way, that is,

$$SS_T = \sum_{i=1}^{2}\sum_{j=1}^{2}\sum_{k=1}^{n} y_{ijk}^2 - \frac{y_{...}^2}{4n} \tag{6-9}$$

In general, SS_T has $4n - 1$ degrees of freedom. The error sum of squares, with $4(n - 1)$ degrees of freedom, is usually computed by subtraction as

$$SS_E = SS_T - SS_A - SS_B - SS_{AB} \tag{6-10}$$

For the experiment in Figure 6-1, we obtain

$$\begin{aligned} SS_T &= \sum_{i=1}^{2}\sum_{j=1}^{2}\sum_{k=1}^{3} y_{ijk}^2 - \frac{y_{...}^2}{4(3)} \\ &= 9398.00 - 9075.00 = 323.00 \end{aligned}$$

and

$$\begin{aligned} SS_E &= SS_T - SS_A - SS_B - SS_{AB} \\ &= 323.00 - 208.33 - 75.00 - 8.33 \\ &= 31.34 \end{aligned}$$

using SS_A, SS_B, and SS_{AB} from Equations 6-8. The complete analysis of variance is summarized in Table 6-1. Based on the P-values, we conclude that the main effects are statistically significant and that there is no interaction between these factors. This confirms our initial interpretation of the data based on the magnitudes of the factor effects.

It is often convenient to write down the treatment combinations in the order (1), a,

Table 6-1 Analysis of Variance for the Experiment in Figure 6-1

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
A	208.33	1	208.33	53.15	0.0001
B	75.00	1	75.00	19.13	0.0024
AB	8.33	1	8.33	2.13	0.1826
Error	31.34	8	3.92		
Total	323.00	11			

b, ab. This is referred to as **standard order** (or Yates' order, for Dr. Frank Yates). Using this standard order, we see that the contrast coefficients used in estimating the effects are

Effects	(1)	a	b	ab
A:	−1	+1	−1	+1
B:	−1	−1	+1	+1
AB:	+1	−1	−1	+1

Note that the contrast coefficients for estimating the interaction effect are just the product of the corresponding coefficients for the two main effects. The contrast coefficient is always either +1 or −1, and a **table of plus and minus signs** such as in Table 6-2 can be used to determine the proper sign for each treatment combination. The column headings in Table 6-2 are the main effects (A and B), the AB interaction, and I, which represents the total or average of the entire experiment. Notice that the column corresponding to I has only plus signs. The row designators are the treatment combinations. To find the contrast for estimating any effect, simply multiply the signs in the appropriate column of the table by the corresponding treatment combination and add. For example, to estimate A, the contrast is $-(1) + a - b + ab$, which agrees with Equation 6-1.

The Regression Model

In a 2^k factorial design, it is easy to express the results of the experiment in terms of a **regression model**. Because the 2^k is just a factorial design, we could also use either an effects or a means model, but the regression model approach is much more natural and intuitive. For the chemical process experiment in Figure 6-1, the regression model is

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

where x_1 is a **coded variable** that represents the reactant concentration and x_2 is a coded variable that represents the amount of catalyst and the β's are regression coefficients.

Table 6-2 Algebraic Signs for Calculating Effects in the 2^2 Design

Treatment Combination	Factorial Effect			
	I	A	B	AB
(1)	+	−	−	+
a	+	+	−	−
b	+	−	+	−
ab	+	+	+	+

The relationship between the **natural variables**, the reactant concentration and the amount of catalyst, and the coded variables is

$$x_1 = \frac{\text{Conc} - (\text{Conc}_{\text{low}} + \text{Conc}_{\text{high}})/2}{(\text{Conc}_{\text{high}} - \text{Conc}_{\text{low}})/2}$$

and

$$x_2 = \frac{\text{Catalyst} - (\text{Catalyst}_{\text{low}} + \text{Catalyst}_{\text{high}})/2}{(\text{Catalyst}_{\text{high}} - \text{Catalyst}_{\text{low}})/2}$$

When the natural variables have only two levels, this coding will produce the familiar ± 1 notation for the levels of the coded variables. To illustrate this for our example, note that

$$x_1 = \frac{\text{Conc} - (15 + 25)/2}{(25 - 15)/2} = \frac{\text{Conc} - 20}{5}$$

Thus, if the concentration is at the high level (Conc = 25%), then $x_1 = +1$; if the concentration is at the low level (Conc = 15%), then $x_1 = -1$. Furthermore,

$$x_2 = \frac{\text{Catalyst} - (1 + 2)/2}{(2 - 1)/2} = \frac{\text{Catalyst} - 1.5}{0.5}$$

Thus, if the catalyst is at the high level (Catalyst = 2 pounds), then $x_2 = +1$; if the catalyst is at the low level (Catalyst = 1 pound), then $x_2 = -1$.

The fitted regression model is

$$\hat{y} = 27.5 + \left(\frac{8.33}{2}\right) x_1 + \left(\frac{-5.00}{2}\right) x_2$$

where the intercept is the grand average of all 12 observations, and the regression coefficients $\hat{\beta}_1$ and $\hat{\beta}_2$ are one-half the corresponding factor effect estimates. The reason that the regression coefficient is one-half the effect estimate is that a regression coefficient measures the effect of a unit change in x on the mean of y, and the effect estimate is based on a two-unit change (from -1 to $+1$). We will show later that this simple method of estimating the regression coefficients is producing **least squares** parameter estimates. Also see the supplemental material for this chapter.

Residuals and Model Adequacy

The regression model can be used to obtain the predicted or fitted value of y at the four points in the design. The residuals are the differences between the observed and fitted values of y. For example, when the reactant concentration is at the low level ($x_1 = -1$) and the catalyst is at the low level ($x_2 = -1$), the predicted yield is

$$\hat{y} = 27.5 + \left(\frac{8.33}{2}\right)(-1) + \left(\frac{-5.00}{2}\right)(-1) = 25.835$$

There are three observations at this treatment combination, and the residuals are

$$e_1 = 28 - 25.835 = 2.165$$
$$e_2 = 25 - 25.835 = -0.835$$
$$e_3 = 27 - 25.835 = 1.165$$

The remaining predicted values and residuals are calculated similarly. For the high level of the reactant concentration and the low level of the catalyst,

$$\hat{y} = 27.5 + \left(\frac{8.33}{2}\right)(+1) + \left(\frac{-5.00}{2}\right)(-1)$$
$$= 34.165$$

and

$$e_4 = 36 - 34.165 = 1.835$$
$$e_5 = 32 - 34.165 = -2.165$$
$$e_6 = 32 - 34.165 = -2.165$$

For the low level of the reactant concentration and the high level of the catalyst,

$$\hat{y} = 27.5 + \left(\frac{8.33}{2}\right)(-1) + \left(\frac{-5.00}{2}\right)(+1)$$
$$= 20.835$$

and

$$e_7 = 18 - 20.835 = -2.835$$
$$e_8 = 19 - 20.835 = -1.835$$
$$e_9 = 23 - 20.835 = 2.165$$

Finally, for the high level of both factors,

$$\hat{y} = 27.5 + \left(\frac{8.33}{2}\right)(+1) + \left(\frac{-5.00}{2}\right)(+1)$$
$$= 29.165$$

and

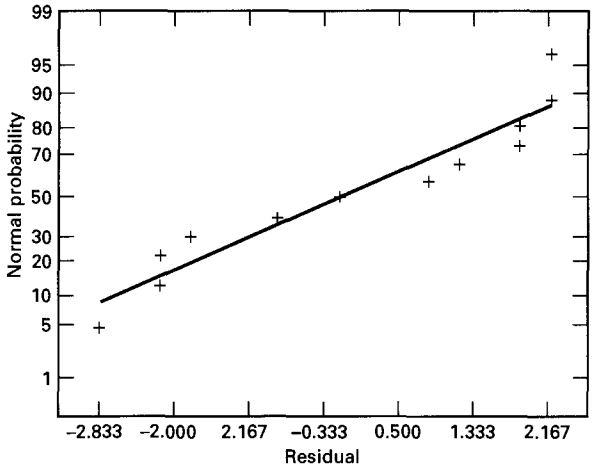
$$e_{10} = 31 - 29.165 = 1.835$$
$$e_{11} = 30 - 29.165 = 0.835$$
$$e_{12} = 29 - 29.165 = -0.165$$

Figure 6-2 (page 226) presents a normal probability plot of these residuals and a plot of the residuals versus the predicted yield. These plots appear satisfactory, so we have no reason to suspect problems with the validity of our conclusions.

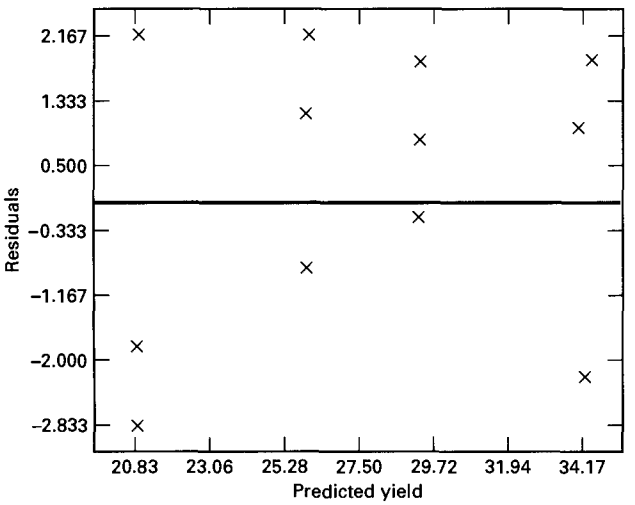
The Response Surface

The regression model

$$\hat{y} = 27.5 + \left(\frac{8.33}{2}\right)x_1 + \left(\frac{-5.00}{2}\right)x_2$$



(*a*) Normal probability plot



(*b*) Residuals versus predicted yield

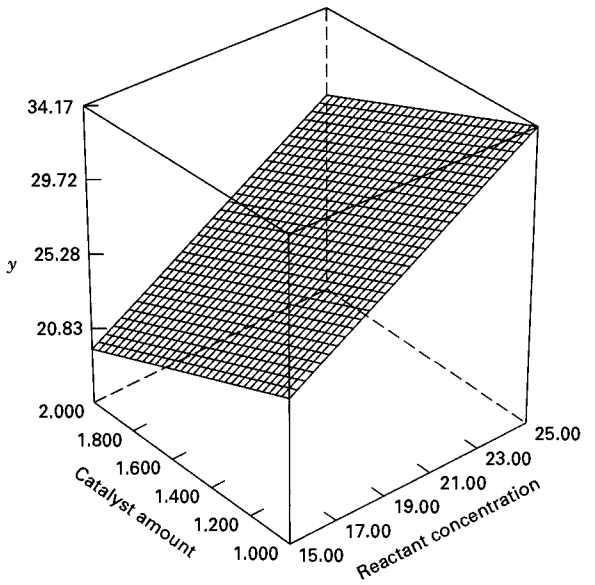
Figure 6-2 Residual plots for the chemical process experiment.

can be used to generate response surface plots. If it is desirable to construct these plots in terms of the **natural factor levels**, then we simply substitute the relationships between the natural and the coded variables that we gave earlier into the regression model, yielding

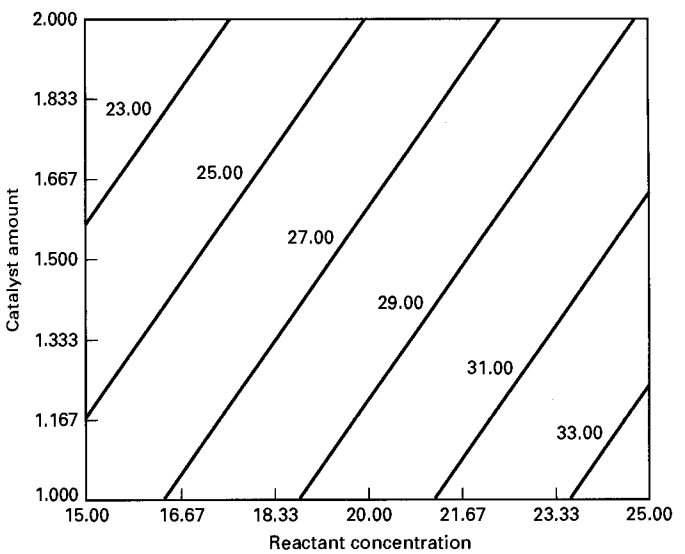
$$\hat{y} = 27.5 + \left(\frac{8.33}{2}\right)\left(\frac{\text{Conc} - 20}{5}\right) + \left(\frac{-5.00}{2}\right)\left(\frac{\text{Catalyst} - 1.5}{0.5}\right)$$

$$= 18.33 + 0.8333\text{Conc} - 5.00\text{Catalyst}$$

Figure 6-3*a* presents the three-dimensional response surface plot of yield from this model, and Figure 6-3*b* is the contour plot. Because the model is **first-order** (that is, it contains only the main effects), the fitted response surface is a plane. From examining



(*a*) Response surface



(*b*) Contour plot

Figure 6-3 Response surface plot and contour plot of yield from the chemical process experiment.

the contour plot, we see that yield increases as reactant concentration increases and catalyst amount decreases. Often, we use a fitted surface such as this to find a **direction of potential improvement** for a process. A formal way to do this, called the **method of steepest ascent**, will be presented in Chapter 11 when we discuss methods for systematically exploring response surfaces.

6-3 THE 2^3 DESIGN

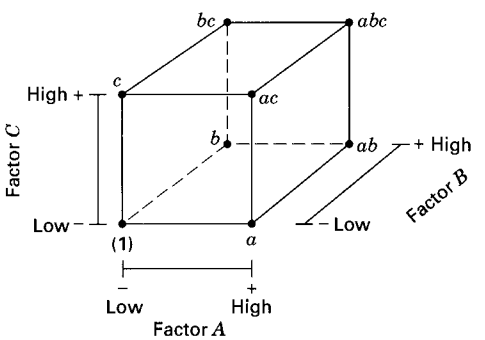
Suppose that three factors, A, B, and C, each at two levels, are of interest. The design is called a **2^3 factorial design** and the eight treatment combinations can now be displayed geometrically as a cube, as shown in Figure 6-4*a*. Using the "+ and −" notation to represent the low and high levels of the factors, we may list the eight runs in the 2^3 design as in Figure 6-4*b*. This is sometimes called the **design matrix**. Extending the label notation discussed in Section 6-2, we write the treatment combinations in standard order as (1), a, b, ab, c, ac, bc, and abc. Remember that these symbols also represent the *total* of all n observations taken at that particular treatment combination.

There are actually three different notations that are widely used for the runs in the 2^k design. The first is the + and − notation, often called the **geometric notation**. The second is the use of lowercase letter labels to identify the treatment combinations. The final notation uses 1 and 0 to denote high and low factor levels, respectively, instead of + and −. These different notations are illustrated below for the 2^3 design:

Run	A	B	C	Labels	A	B	C
1	−	−	−	(1)	0	0	0
2	+	−	−	a	1	0	0
3	−	+	−	b	0	1	0
4	+	+	−	ab	1	1	0
5	−	−	+	c	0	0	1
6	+	−	+	ac	1	0	1
7	−	+	+	bc	0	1	1
8	+	+	+	abc	1	1	1

There are seven degrees of freedom between the eight treatment combinations in the 2^3 design. Three degrees of freedom are associated with the main effects of A, B, and C. Four degrees of freedom are associated with interactions; one each with AB, AC, and BC and one with ABC.

Consider estimating the main effects. First, consider estimating the main effect A. The effect of A when B and C are at the low level is $[a - (1)]/n$. Similarly, the effect of A when B is at the high level and C is at the low level is $[ab - b]/n$. The effect of A



(*a*) Geometric view

Run	Factor A	B	C
1	−	−	−
2	+	−	−
3	−	+	−
4	+	+	−
5	−	−	+
6	+	−	+
7	−	+	+
8	+	+	+

(*b*) The design matrix

Figure 6-4 The 2^3 factorial design.

when C is at the high level and B is at the low level is $[ac - c]/n$. Finally, the effect of A when both B and C are at the high level is $[abc - bc]/n$. Thus, the average effect of A is just the average of these four, or

$$A = \frac{1}{4n}[a - (1) + ab - b + ac - c + abc - bc] \tag{6-11}$$

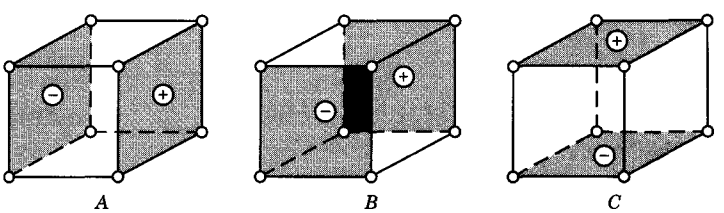
This equation can also be developed as a contrast between the four treatment combinations in the right face of the cube in Figure 6-5*a* (where A is at the high level) and the four in the left face (where A is at the low level). That is, the A effect is just the average of the four runs where A is at the high level ($\bar{y}_{A^+}$) minus the average of the four runs where A is at the low level ($\bar{y}_{A^-}$), or

$$\begin{aligned} A &= \bar{y}_{A^+} - \bar{y}_{A^-} \\ &= \frac{a + ab + ac + abc}{4n} - \frac{(1) + b + c + bc}{4n} \end{aligned}$$

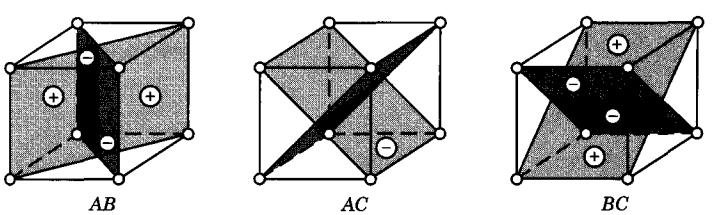
This equation can be rearranged as

$$A = \frac{1}{4n}[a + ab + ac + abc - (1) - b - c - bc]$$

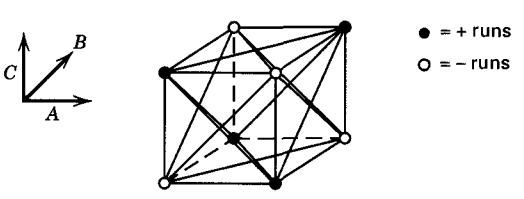
which is identical to Equation 6-11.



(*a*) Main effects



(*b*) Two-factor interaction



(*c*) Three-factor interaction

Figure 6-5 Geometric presentation of contrasts corresponding to the main effects and interactions in the 2^3 design.

In a similar manner, the effect of B is the difference in averages between the four treatment combinations in the front face of the cube and the four in the back. This yields

$$\begin{aligned} B &= \bar{y}_{B^+} - \bar{y}_{B^-} \\ &= \frac{1}{4n}[b + ab + bc + abc - (1) - a - c - ac] \end{aligned} \tag{6-12}$$

The effect of C is the difference in averages between the four treatment combinations in the top face of the cube and the four in the bottom, that is,

$$\begin{aligned} C &= \bar{y}_{C^+} - \bar{y}_{C^-} \\ &= \frac{1}{4n}[c + ac + bc + abc - (1) - a - b - ab] \end{aligned} \tag{6-13}$$

The two-factor interaction effects may be computed easily. A measure of the AB interaction is the difference between the average A effects at the two levels of B. By convention, one-half of this difference is called the AB interaction. Symbolically,

B	Average A Effect
High (+)	$\dfrac{[(abc - bc) + (ab - b)]}{2n}$
Low (−)	$\dfrac{\{(ac - c) + [a - (1)]\}}{2n}$
Difference	$\dfrac{[abc - bc + ab - b - ac + c - a + (1)]}{2n}$

Because the AB interaction is one-half of this difference,

$$AB = \frac{[abc - bc + ab - b - ac + c - a + (1)]}{4n} \tag{6-14}$$

We could write Equation 6-14 as follows:

$$AB = \frac{abc + ab + c + (1)}{4n} - \frac{bc + b + ac + a}{4n}$$

In this form, the AB interaction is easily seen to be the difference in averages between runs on two diagonal planes in the cube in Figure 6-5*b*. Using similar logic and referring to Figure 6-5*b*, the AC and BC interactions are

$$AC = \frac{1}{4n}[(1) - a + b - ab - c + ac - bc + abc] \tag{6-15}$$

and

$$BC = \frac{1}{4n}[(1) + a - b - ab - c - ac + bc + abc] \tag{6-16}$$

The ABC interaction is defined as the average difference between the AB interaction for the two different levels of C. Thus,

$$ABC = \frac{1}{4n}\{[abc - bc] - [ac - c] - [ab - b] + [a - (1)]\}$$

$$= \frac{1}{4n}[abc - bc - ac + c - ab + b + a - (1)] \tag{6-17}$$

As before, we can think of the ABC interaction as the difference in two averages. If the runs in the two averages are isolated, they define the vertices of the two tetrahedra that comprise the cube in Figure 6-5*c*.

In Equations 6-11 through 6-17, the quantities in brackets are **contrasts** in the treatment combinations. A table of plus and minus signs can be developed from the contrasts and is shown in Table 6-3. Signs for the main effects are determined by associating a plus with the high level and a minus with the low level. Once the signs for the main effects have been established, the signs for the remaining columns can be obtained by multiplying the appropriate preceding columns, row by row. For example, the signs in the AB column are the product of the A and B column signs in each row. The contrast for any effect can be obtained easily from this table.

Table 6-3 has several interesting properties: (1) Except for column I, every column has an equal number of plus and minus signs. (2) The sum of the products of the signs in any two columns is zero. (3) Column I multiplied times any column leaves that column unchanged. That is, I is an **identity element**. (4) The product of any two columns yields a column in the table. For example, $A \times B = AB$, and

$$AB \times B = AB^2 = A$$

We see that the exponents in the products are formed by using **modulus 2** arithmetic. (That is, the exponent can only be 0 or 1; if it is greater than 1, it is reduced by multiples of 2 until it is either 0 or 1.) All of these properties are implied by the orthogonality of the contrasts used to estimate the effects.

Sums of squares for the effects are easily computed, because each effect has a corresponding single-degree-of-freedom contrast. In the 2^3 design with n replicates, the sum of squares for any effect is

$$SS = \frac{(\text{Contrast})^2}{8n} \tag{6-18}$$

Table 6-3 Algebraic Signs for Calculating Effects in the 2^3 Design

Treatment Combination	Factorial Effect							
	I	A	B	AB	C	AC	BC	ABC
(1)	+	−	−	+	−	+	+	−
a	+	+	−	−	−	−	+	+
b	+	−	+	−	−	+	−	+
ab	+	+	+	+	−	−	−	−
c	+	−	−	+	+	−	−	+
ac	+	+	−	−	+	+	−	−
bc	+	−	+	−	+	−	+	−
abc	+	+	+	+	+	+	+	+

EXAMPLE 6-1

Recall Example 5-3, which presented a study on the effect of percentage of carbonation, operating pressure, and line speed on the fill height of a carbonated beverage. Suppose that only two levels of carbonation are used so that the experiment is a 2^3 factorial design with two replicates. The data, deviations from the target fill height, are shown in Table 6-4, and the design is shown geometrically in Figure 6-6.

Using the totals under the treatment combinations shown in Table 6-4, we may estimate the factor effects as follows:

$$A = \frac{1}{4n}[a - (1) + ab - b + ac - c + abc - bc]$$
$$= \frac{1}{8}[1 - (-4) + 5 - (-1) + 3 - (-1) + 11 - 2]$$
$$= \frac{1}{8}[24] = 3.00$$
$$B = \frac{1}{4n}[b + ab + bc + abc - (1) - a - c - ac]$$
$$= \frac{1}{8}[-1 + 5 + 2 + 11 - (-4) - 1 - (-1) - 3]$$
$$= \frac{1}{8}[18] = 2.25$$
$$C = \frac{1}{4n}[c + ac + bc + abc - (1) - a - b - ab]$$
$$= \frac{1}{8}[-1 + 3 + 2 + 11 - (-4) - 1 - (-1) - 5]$$
$$= \frac{1}{8}[14] = 1.75$$
$$AB = \frac{1}{4n}[ab - a - b + (1) + abc - bc - ac + c]$$
$$= \frac{1}{8}[5 - 1 - (-1) + (-4) + 11 - 2 - 3 + (-1)]$$
$$= \frac{1}{8}[6] = 0.75$$

Table 6-4 The Fill Height Experiment, Example 6-1

	Coded Factors			Fill Height Deviation		Factor Levels		
Run	A	B	C	Replicate 1	Replicate 2		Low (−1)	High (+1)
1	−1	−1	−1	−3	−1	A (%)	10	12
2	1	−1	−1	0	1	B (psi)	25	30
3	−1	1	−1	−1	0	C (b/min)	200	250
4	1	1	−1	2	3			
5	−1	−1	1	−1	0			
6	1	−1	1	2	1			
7	−1	1	1	1	1			
8	1	1	1	6	5			

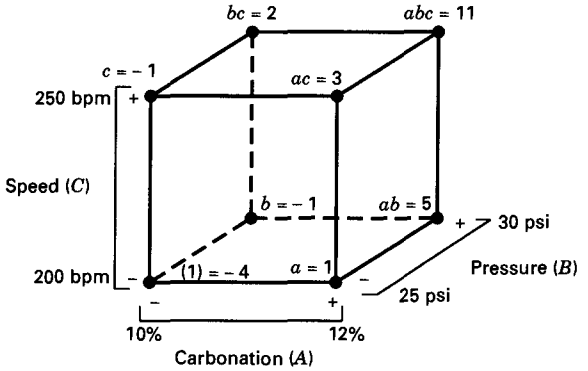


Figure 6-6 The 2^3 design for the fill height deviation experiment for Example 6-1.

$$AC = \frac{1}{4n}[(1) - a + b - ab - c + ac - bc + abc]$$

$$= \frac{1}{8}[-4 - 1 + (-1) - 5 - (-1) + 3 - 2 + 11]$$

$$= \frac{1}{8}[2] = 0.25$$

$$BC = \frac{1}{4n}[(1) + a - b - ab - c - ac + bc + abc]$$

$$= \frac{1}{8}[-4 + 1 - (-1) - 5 - (-1) - 3 + 2 + 11]$$

$$= \frac{1}{8}[4] = 0.50$$

and

$$ABC = \frac{1}{4n}[abc - bc - ac + c - ab + b + a - (1)]$$

$$= \frac{1}{8}[11 - 2 - 3 + (-1) - 5 + (-1) + 1 - (-4)]$$

$$= \frac{1}{8}[4] = 0.50$$

The largest effects are for carbonation ($A = 3.00$), pressure ($B = 2.25$), speed ($C = 1.75$) and the carbonation–pressure interaction ($AB = 0.75$), although the interaction effect does not appear to have as large an impact on fill height deviation as the main effects.

The sums of squares are calculated from Equation 6-18 as follows:

$$SS_A = \frac{(24)^2}{16} = 36.00$$

$$SS_B = \frac{(18)^2}{16} = 20.25$$

$$SS_C = \frac{(14)^2}{16} = 12.25$$

Table 6-5 Effect Estimate Summary for Example 6-1

Factor	Effect Estimate	Sum of Squares	Percent Contribution
A	3.00	36.00	46.1538
B	2.25	20.25	25.9615
C	1.75	12.25	15.7051
AB	0.75	2.25	2.88462
AC	0.25	0.25	0.320513
BC	0.50	1.00	1.28205
ABC	0.50	1.00	1.28205
Pure Error		5.00	6.41026
Total		78.00	

$$SS_{AB} = \frac{(6)^2}{16} = 2.25$$

$$SS_{AC} = \frac{(2)^2}{16} = 0.25$$

$$SS_{BC} = \frac{(4)^2}{16} = 1.00$$

and

$$SS_{ABC} = \frac{(4)^2}{16} = 1.00$$

The total sum of squares is $SS_T = 78.00$, and by subtraction, $SS_E = 5.00$. Table 6-5 summarizes the effect estimates and sums of squares. The column labeled "percent contribution" measures the percentage contribution of each model term to the total sum of squares. The percentage contribution is often a rough but effective guide to the relative importance of each model term. Note that the main effects really dominate this process, accounting for over 87 percent of the total variability, whereas the *AB* interaction accounts for less than 3 percent.

The analysis of variance in Table 6-6 may be used to confirm the magnitude of these effects. From Table 6-6 we note that the main effects are highly significant (all have very

Table 6-6 Analysis of Variance for the Fill Height Data

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	*P*-Value
Percent carbonation (*A*)	36.00	1	36.00	57.60	<0.0001
Pressure (*B*)	20.25	1	20.25	32.40	0.0005
Line speed (*C*)	12.25	1	12.25	19.60	0.0022
AB	2.25	1	2.25	3.60	0.0943
AC	0.25	1	0.25	0.40	0.5447
BC	1.00	1	1.00	1.60	0.2415
ABC	1.00	1	1.00	1.60	0.2415
Error	5.00	8	0.625		
Total	78.00	15			

small P-values). The AB interaction is significant at about the 10 percent level; thus there is some mild interaction between carbonation and pressure.

The reader may wish to refer to Example 5-3 for the practical interpretation of this experiment. The process developers decided to run the process at low pressure and high line speed and to reduce the variability in carbonation by controlling the temperature more precisely. This resulted in a substantial reduction in the deviation of fill height from the target value.

The Regression Model and Response Surface

The regression model for predicting fill height deviation is

$$\begin{aligned}\hat{y} &= \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \hat{\beta}_{12} x_1 x_2 \\ &= 1.00 + \left(\frac{3.00}{2}\right) x_1 + \left(\frac{2.25}{2}\right) x_2 + \left(\frac{1.75}{2}\right) x_3 + \left(\frac{0.75}{2}\right) x_1 x_2,\end{aligned}$$

where the coded variables x_1, x_2, and x_3 represent A, B, and C, respectively. The $x_1 x_2$ term is the AB interaction. Residuals can be obtained as the difference between observed and predicted fill height deviations. We leave the analysis of these residuals as an exercise for the reader.

Figure 6-7 (page 236) presents the response surface and contour plot for fill height deviation obtained from the regression model, assuming that line speed is at the high level ($x_3 = 1$). Notice that because the model contains interaction, the contour lines of constant fill height deviation are curved (or the response surface is a "twisted" plane). It is desirable to operate this filling process so that fill deviation is as close to zero as possible. The contour plot shows that if line speed is at the high level, then there are several combinations of pressure and carbonation level that will satisfy this objective. However, it will be necessary to control both of these variables very precisely.

Computer Solution

There are many statistics software packages that will set up and analyze two-level factorial designs. The output from one of these computer programs, Design-Expert, is shown in Table 6-7 (pages 237, 238). In the upper part of the table an analysis of variance for the full model is presented. The format of this presentation is somewhat different from the results given in Table 6-6. Notice that the first line of the analysis of variance is an overall summary for the full model (all main effects and interactions), and the model sum of squares is

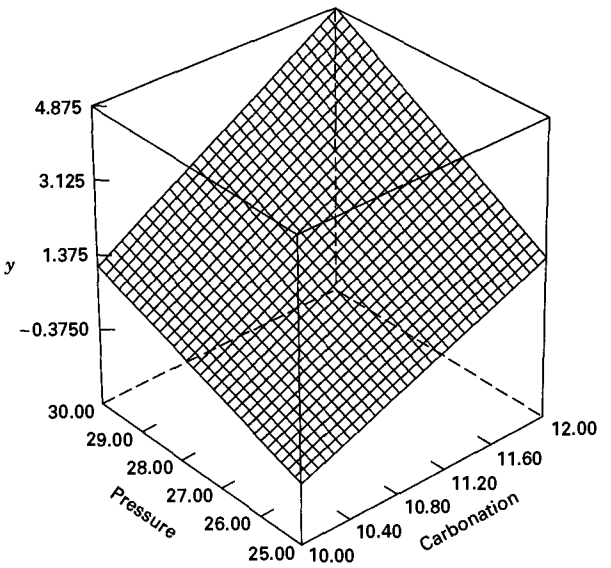
$$\begin{aligned}SS_{\text{Model}} &= SS_A + SS_B + SS_C + SS_{AB} + SS_{AC} + SS_{BC} + SS_{ABC} \\ &= 73.0\end{aligned}$$

Thus the statistic

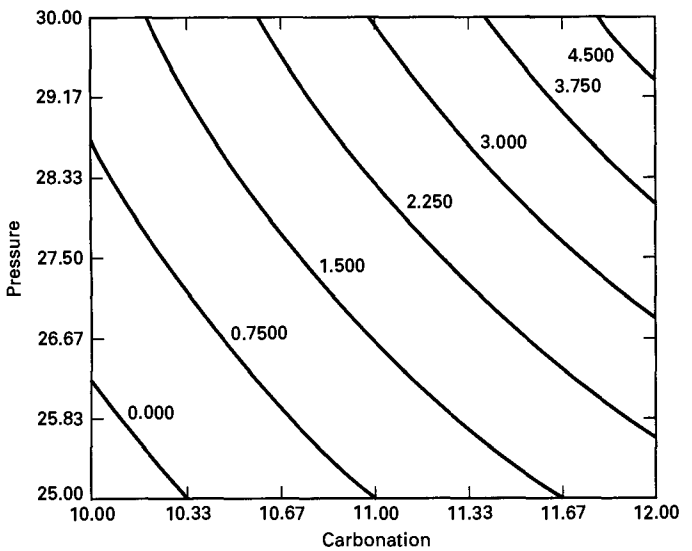
$$F_0 = \frac{MS_{\text{Model}}}{MS_E} = \frac{10.43}{0.63} = 16.69$$

is testing the hypotheses

$$\begin{aligned}&H_0: \beta_1 = \beta_2 = \beta_3 = \beta_{12} = \beta_{13} = \beta_{23} = \beta_{123} = 0 \\ &H_1: \text{at least one } \beta \neq 0\end{aligned}$$



(*a*) The response surface



(*b*) The contour plot

Figure 6-7 Response surface and contour plot of fill height deviation with speed at the high level (250 bpm), Example 6-1.

Table 6-7 Design-Expert Output for Example 6-1

Response: Fill Deviation in Height
ANOVA for Selected Factorial Model
Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Model	73.00	7	10.43	16.69	0.0003	significant
A	*36.00*	*1*	*36.00*	*57.60*	*<0.0001*	
B	*20.25*	*1*	*20.25*	*32.40*	*0.0005*	
C	*12.25*	*1*	*12.25*	*19.60*	*0.0022*	
AB	*2.25*	*1*	*2.25*	*3.60*	*0.0943*	
AC	*0.25*	*1*	*0.25*	*0.40*	*0.5447*	
BC	*1.00*	*1*	*1.00*	*1.60*	*0.2415*	
ABC	*1.00*	*1*	*1.00*	*1.60*	*0.2415*	
Residual	5.00	8	0.63			
Lack of Fit	*0.000*	*0*				
Pure Error	*5.00*	*8*	*0.63*			
Cor Total	78.00	15				

Std. Dev.	0.79	R-Squared	0.9359
Mean	1.00	Adj R-Squared	0.8798
C.V.	79.06	Pred R-Squared	0.7436
PRESS	20.00	Adeq Precision	13.416

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High	VIF
Intercept	1.00	1	0.20	0.54	1.46	
A-Carbonation	1.50	1	0.20	1.04	1.96	1.00
B-Pressure	1.13	1	0.20	0.67	1.58	1.00
C-Speed	0.88	1	0.20	0.42	1.33	1.00
AB	0.38	1	0.20	−0.081	0.83	1.00
AC	0.13	1	0.20	−0.33	0.58	1.00
BC	0.25	1	0.20	−0.21	0.71	1.00
ABC	0.25	1	0.20	−0.21	0.71	1.00

Final Equation in Terms of Coded Factors:

Fill Deviation =
+1.00
+1.50 *A
+1.13 *B
+0.88 *C
+0.38 *A *B
+0.13 *A *C
+0.25 *B *C
+0.25 *A *B *C

Final Equation in Terms of Actual Factors:

Fill Deviation =
−225.50000
+21.00000 *Carbonation
+7.80000 *Pressure
+1.08000 *Speed
−0.75000 *Carbonation *Pressure
−0.10500 *Carbonation *Speed
−0.040000 *Pressure *Speed
+4.00000E-00: *Carbonation *Pressure *Speed

Reduced Model:
Response: Fill Deviation in Height
ANOVA for Selected Factorial Model
Analysis of variance table [Partial sum of squares]

Table 6-7 (continued)

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Model	70.75	4	17.69	26.84	<0.0001	significant
A	*36.00*	*1*	*36.00*	*54.62*	*<0.0001*	
B	*20.25*	*1*	*20.25*	*30.72*	*0.0002*	
C	*12.25*	*1*	*12.25*	*18.59*	*0.0012*	
AB	*2.25*	*1*	*2.25*	*3.41*	*0.0917*	
Residual	7.25	11	0.66			
Lack of Fit	*2.25*	*3*	*0.75*	*1.20*	*0.3700*	*not significant*
Pure Error	*5.00*	*8*	*0.63*			
Cor Total	78.00	15				

Std. Dev.	0.81	R-Squared	0.9071
Mean	1.00	Adj R-Squared	0.8733
C.V.	81.18	Pred R-Squared	0.8033
PRESS	15.34	Adeq Precision	15.424

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High	VIF
Intercept	1.00	1	0.20	0.55	1.45	
A-Carbonation	1.50	1	0.20	1.05	1.95	1.00
B-Pressure	1.13	1	0.20	0.68	1.57	1.00
C-Speed	0.88	1	0.20	0.43	1.32	1.00
AB	0.38	1	0.20	−0.072	0.82	1.00

Final Equation in Terms of Coded Factors:

Fill Deviation =
+1.00
+1.50 *A
+1.13 *B
+0.88 *C
+0.38 *A *B

Final Equation in Terms of Actual Factors:

Fill Deviation =
+9.62500
−2.62500 *Carbonation
−1.20000 *Pressure
+0.035000 *Speed
+0.15000 *Carbonation *Pressure

Diagnostics Case Statistics

Standard Order	Actual Value	Predicted Value	Residual	Leverage	Student Residual	Cook's Distance	Outlier t
1	−3.00	−2.13	−0.88	0.313	−1.300	0.154	−1.347
2	−1.00	−2.13	1.13	0.313	1.671	0.254	1.845
3	0.000	0.12	−0.12	0.313	−0.186	0.003	−0.177
4	1.00	0.12	0.88	0.313	1.300	0.154	1.347
5	−1.00	−0.63	−0.38	0.313	−0.557	0.028	−0.539
6	0.000	−0.63	0.63	0.313	0.928	0.078	0.922
7	2.00	3.13	−1.13	0.313	−1.671	0.254	−1.845
8	3.00	3.13	−0.13	0.313	−0.186	0.003	−0.177
9	−1.00	−0.37	−0.63	0.313	−0.928	0.078	−0.922
10	0.000	−0.37	0.37	0.313	0.557	0.028	0.539
11	2.00	1.88	0.13	0.313	0.186	0.003	0.177
12	1.00	1.88	−0.88	0.313	−1.300	0.154	−1.347
13	1.00	1.13	−0.13	0.313	−0.186	0.003	−0.177
14	1.00	1.13	−0.13	0.313	−0.186	0.003	−0.177
15	6.00	4.88	1.13	0.313	1.671	0.254	1.845
16	5.00	4.88	0.13	0.313	0.186	0.003	0.177

Because F_0 is large, we would conclude that at least one variable has a nonzero effect. Then each individual factorial effect is tested for significance using the F statistic. These results agree with Table 6-6.

Below the full model analysis of variance, several R^2 statistics are presented. The ordinary R^2 is

$$R^2 = \frac{SS_{\text{Model}}}{SS_{\text{Total}}} = \frac{73.00}{78.00} = 0.9359$$

and it measures the proportion of total variability explained by the model. A potential problem with this statistic is that it always increases as factors are added to the model, even if these factors are not significant. The **adjusted** R^2 statistic, defined as

$$R^2_{\text{Adj}} = 1 - \frac{SS_E/df_E}{SS_{\text{Total}}/df_{\text{Total}}} = 1 - \frac{5.00/8}{78.00/15} = 0.8798$$

is a statistic that is adjusted for the "size" of the model; that is, the number of factors. The adjusted R^2 can actually decrease if nonsignificant terms are added to a model. The PRESS statistic is a measure of how well the model will predict new data (PRESS is actually an acronym for Prediction Error Sum of Squares, and it is computed from the prediction errors obtained by predicting the ith data point with a model that includes all observations *except* the ith one.). A model with a small value of PRESS indicates that the model is likely to be a good predictor. The "Prediction R^2" statistic is computed as

$$R^2_{\text{Pred}} = 1 - \frac{\text{PRESS}}{SS_{\text{Total}}} = 1 - \frac{20.00}{78.00} = 0.7436$$

This indicates that the full model would be expected to explain about 74 percent of the variability in new data.

The next portion of the output presents the regression coefficient for each model term and the **standard error** of each coefficient, defined as

$$se(\hat{\beta}) = \sqrt{V(\hat{\beta})} = \sqrt{\frac{MS_E}{n2^k}} = \sqrt{\frac{0.625}{2(8)}} = 0.20$$

The 95 percent confidence intervals on each regression coefficient are computed from

$$\hat{\beta} - t_{0.025,N-p}se(\hat{\beta}) \leq \beta \leq \hat{\beta} + t_{0.025,N-p}se(\hat{\beta})$$

where the degrees of freedom on t are the number of degrees of freedom for error; that is, N is the total number of runs in the experiment (16), and p is the number of model parameters (8). The full model in terms of both the coded variables and the natural variables is also presented.

The last part of the display in Table 6-7 illustrates the output following removal of the nonsignificant interaction terms. This reduced model now contains only the main effects A, B, and C, and the AB interaction. The **error** or **residual** sum of squares is now composed of a **pure error** component arising from the replication of the eight corners of the cube, and a **lack of fit** component consisting of the sums of squares for the interactions that were dropped from the model (BC, AC, and ABC). Once again, the regression model representation of the experimental results is given in terms of both

coded and natural variables. The proportion of total variability in fill height deviation that is explained by this model is

$$R^2 = \frac{SS_{\text{Model}}}{SS_{\text{Total}}} = \frac{70.75}{78.00} = 0.9071$$

which is smaller than the R^2 for the full model. Notice, however, that the adjusted R^2 for the reduced model has changed only slightly from the adjusted R^2 for the full model, and PRESS for the reduced model is considerably smaller, leading to a larger value of R^2_{Pred} for the reduced model. Clearly removing the nonsignificant terms from the full model has produced a final model that is likely to function more effectively as a predictor of new data. Notice that the confidence intervals on the regression coefficients for the reduced model are slightly shorter than the corresponding confidence intervals for the full model.

The last part of the output presents the residuals from the reduced model. Design-Expert will also construct all of the residual plots that we have previously discussed.

Other Methods for Judging the Significance of Effects

The analysis of variance is a formal way to determine which factor effects are nonzero. There are several other methods that are useful. Below, we show how to calculate the **standard error of the effects** and use these standard errors to construct **confidence intervals** on the effects. Another method, which we will illustrate in Section 6-5, uses **normal probability plots** to assess the importance of the effects.

The standard error of an effect is easy to find. If we assume that there are n replicates at each of the 2^k runs in the design, and if $y_{i1}, y_{i2}, \ldots, y_{in}$ are the observations at the ith run, then

$$S_i^2 = \frac{1}{n-1}\sum_{j=1}^{n}(y_{ij} - \bar{y}_i)^2 \qquad i = 1, 2, \ldots, 2^k$$

is an estimate of the variance at the ith run. The 2^k variance estimates can be combined to give an overall variance estimate:

$$S^2 = \frac{1}{2^k(n-1)}\sum_{i=1}^{2^k}\sum_{j=1}^{n}(y_{ij} - \bar{y}_i)^2 \tag{6-19}$$

This is also the variance estimate given by the error mean square in the analysis of variance. The *variance* of each effect estimate is

$$\begin{aligned} V(\text{Effect}) &= V\left(\frac{\text{Contrast}}{n2^{k-1}}\right) \\ &= \frac{1}{(n2^{k-1})^2}V(\text{Contrast}) \end{aligned}$$

Each contrast is a linear combination of 2^k treatment totals, and each total consists of n observations. Therefore,

$$V(\text{Contrast}) = n2^k\sigma^2$$

and the variance of an effect is

$$V(\text{Effect}) = \frac{1}{(n2^{k-1})^2} n2^k\sigma^2$$
$$= \frac{1}{n2^{k-2}} \sigma^2$$
$$= \frac{2\sigma}{\sqrt{n2^k}}$$

The estimated standard error would be found by taking the square root of this last expression and replacing σ^2 by its estimate S^2:

$$se(\text{Effect}) = \frac{2S}{\sqrt{n2^k}} \tag{6-20}$$

Notice that the standard error of an effect is twice the standard error of an estimated regression coefficient in the regression model for the 2^k design (see the Design-Expert computer output for Example 6-1).

The $100(1 - \alpha)$ percent confidence intervals on the effects are computed from Effect $\pm t_{\alpha/2,N-p} se(\text{Effect})$, where the degrees of freedom on t are just the error or residual degrees of freedom ($N - p$ = total number of runs − number of model parameters).

To illustrate this method, consider the fill height deviation experiment in Example 6-1. The mean square error is $MS_E = 0.625$. Therefore, the standard error of each effect is (using $S^2 = MS_E$)

$$se(\text{Effect}) = \frac{2S}{\sqrt{n2^k}}$$
$$= \frac{2\sqrt{0.625}}{\sqrt{2(2^3)}}$$
$$= 0.40$$

Now $t_{0.025,8} = 2.31$ and $t_{0.025,8}\ se(\text{Effect}) = 2.31(0.40) = 0.92$, so approximate 95 percent confidence intervals on the factor effects are

$$\begin{aligned} A&: \quad 3.00 \pm 0.92 \\ B&: \quad 2.25 \pm 0.92 \\ C&: \quad 1.75 \pm 0.92 \\ AB&: \quad 0.75 \pm 0.92 \\ AC&: \quad 0.25 \pm 0.92 \\ BC&: \quad 0.50 \pm 0.92 \\ ABC&: \quad 0.50 \pm 0.92 \end{aligned}$$

This analysis indicates that A, B, and C are important factors, because they are the only factor effect estimates for which the approximate 95 percent confidence intervals do not include zero.

Dispersion Effects

The process engineer working on the filling process was also interested in **dispersion effects**; that is, do any of the factors affect variability in fill height deviation from run

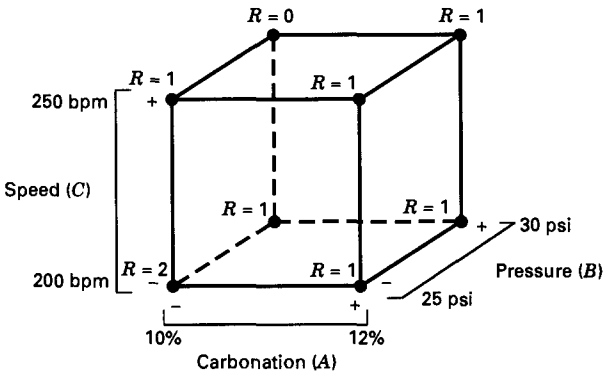


Figure 6-8 Ranges of fill height deviation for Example 6-1.

to run? One way to answer the question is to look at the **range** of fill height deviations for each of the eight runs in the 2^3 design. These ranges are plotted on the cube in Figure 6-8. Notice that the ranges are about the same for all eight runs in the design. Consequently, there is no strong evidence indicating that some of the process variables directly affect the variability in fill height deviation in the process.

6-4 THE GENERAL 2^k DESIGN

The methods of analysis that we have presented thus far may be generalized to the case of a **2^k factorial design**, that is, a design with k factors each at two levels. The statistical model for a 2^k design would include k main effects, $\binom{k}{2}$ two-factor interactions, $\binom{k}{3}$ three-factor interactions, . . . , and one k-factor interaction. That is, for a 2^k design the complete model would contain $2^k - 1$ effects. The notation introduced earlier for treatment combinations is also used here. For example, in a 2^5 design *abd* denotes the treatment combination with factors A, B, and D at the high level and factors C and E at the low level. The treatment combinations may be written in **standard order** by introducing the factors one at a time, with each new factor being successively combined with those that precede it. For example, the standard order for a 2^4 design is (1), *a*, *b*, *ab*, *c*, *ac*, *bc*, *abc*, *d*, *ad*, *bd*, *abd*, *cd*, *acd*, *bcd*, and *abcd*.

The general approach to the statistical analysis of the 2^k design is summarized in Table 6-8. As we have indicated previously, a computer software package is usually employed in this analysis process.

The sequence of steps in Table 6-8 should, by now, be familiar. The first step is to estimate factor effects and examine their signs and magnitudes. This gives the experi-

Table 6-8 Analysis Procedure for a 2^k Design

1. Estimate factor effects
2. Form initial model
3. Perform statistical testing
4. Refine model
5. Analyze residuals
6. Interpret results

menter preliminary information regarding which factors and interactions may be important, and in which directions these factors should be adjusted to improve the response. In forming the initial model for the experiment, we usually choose the **full model**, that is, all main effects and interactions, provided that at least one of the design points has been replicated (in the next section, we discuss a modification to this step). Then in step 3, we use the analysis of variance to formally test for significance of main effects and interaction. Table 6-9 shows the general form of an analysis of variance for a 2^k factorial design with n replicates. Step 4, refine the model, usually consists of removing any nonsignificant variables from the full model. Step 5 is the usual residual analysis to check for model adequacy and to check assumptions. Sometimes model refinement will occur after residual analysis, if we find that the model is inadequate or assumptions are badly violated. The final step usually consists of graphical analysis—either main effect or interaction plots, or response surface and contour plots.

Although the calculations described above are almost always done with a computer, occasionally it is necessary to manually calculate an effect estimate or sum of squares for an effect. To estimate an effect or to compute the sum of squares for an effect, we must first determine the contrast associated with that effect. This can always be done by using a table of plus and minus signs, such as Table 6-2 or Table 6-3. However, for large values of k this is awkward, and we can use an alternate method. In general, we determine the contrast for effect $AB \cdots K$ by expanding the right-hand side of

$$\text{Contrast}_{AB\cdots K} = (a \pm 1)(b \pm 1) \cdots (k \pm 1) \tag{6-21}$$

Table 6-9 Analysis of Variance for a 2^k Design

Source of Variation	Sum of Squares	Degrees of Freedom
k main effects		
A	SS_A	1
B	SS_B	1
⋮	⋮	⋮
K	SS_K	1
$\binom{k}{2}$ two-factor interactions		
AB	SS_{AB}	1
AC	SS_{AC}	1
⋮	⋮	⋮
JK	SS_{JK}	1
$\binom{k}{3}$ three-factor interactions		
ABC	SS_{ABC}	1
ABD	SS_{ABD}	1
⋮	⋮	⋮
IJK	SS_{IJK}	1
⋮	⋮	⋮
$\binom{k}{k} = 1$ k-factor interaction		
$ABC \cdots K$	$SS_{ABC\cdots K}$	1
Error	SS_E	$2^k(n-1)$
Total	SS_T	$n2^k - 1$

In expanding Equation 6-21, ordinary algebra is used with "1" being replaced by (1) in the final expression. The sign in each set of parentheses is negative if the factor is included in the effect and positive if the factor is not included.

To illustrate the use of Equation 6-21, consider a 2^3 factorial design. The contrast for AB would be

$$\begin{aligned}\text{Contrast}_{AB} &= (a - 1)(b - 1)(c + 1) \\ &= abc + ab + c + (1) - ac - bc - a - b\end{aligned}$$

As a further example, in a 2^5 design, the contrast for $ABCD$ would be

$$\begin{aligned}\text{Contrast}_{ABCD} &= (a - 1)(b - 1)(c - 1)(d - 1)(e + 1) \\ &= abcde + cde + bde + ade + bce \\ &\quad + ace + abe + e + abcd + cd + bd \\ &\quad + ad + bc + ac + ab + (1) - a - b - c \\ &\quad - abc - d - abd - acd - bcd - ae \\ &\quad - be - ce - abce - de - abde - acde - bcde\end{aligned}$$

Once the contrasts for the effects have been computed, we may estimate the effects and compute the sums of squares according to

$$AB \cdots K = \frac{2}{n2^k}(\text{Contrast}_{AB\cdots K}) \tag{6-22}$$

and

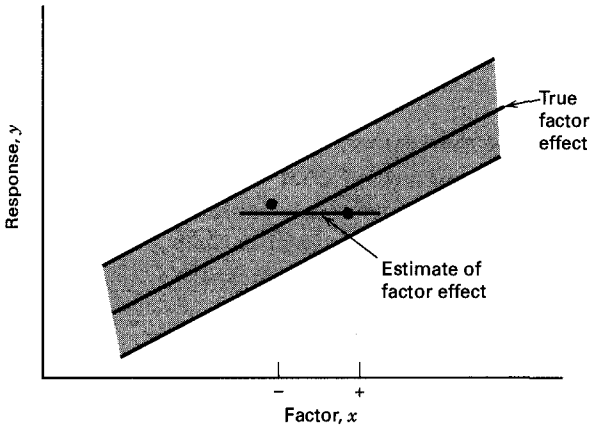
$$SS_{AB\cdots K} = \frac{1}{n2^k}(\text{Contrast}_{AB\cdots K})^2 \tag{6-23}$$

respectively, where n denotes the number of replicates. There is also a tabular algorithm due to Dr. Frank Yates that can occasionally be useful for manual calculation of the effect estimates and the sums of squares. Refer to the supplemental text material for this chapter.

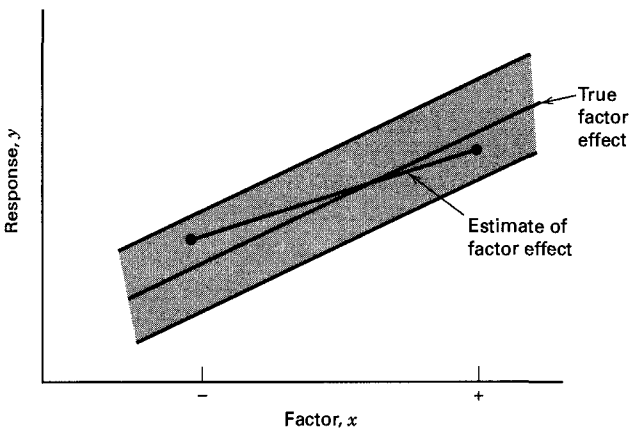
6-5 A SINGLE REPLICATE OF THE 2^k DESIGN

For even a moderate number of factors, the total number of treatment combinations in a 2^k factorial design is large. For example, a 2^5 design has 32 treatment combinations, a 2^6 design has 64 treatment combinations, and so on. Because resources are usually limited, the number of replicates that the experimenter can employ may be restricted. Frequently, available resources only allow a **single replicate** of the design to be run, unless the experimenter is willing to omit some of the original factors.

An obvious risk when conducting an experiment that has only one run at each test combination is that we may be fitting a model to noise. That is, if the response y is highly variable, misleading conclusions may result from the experiment. The situation is illustrated in Figure 6-9*a*. In this figure, the straight line represents the true factor effect. However, because of the random variability present in the response variable (represented by the shaded band), the experimenter actually obtains the two measured responses represented by the dark dots. Consequently, the estimated factor effect is close to zero, and the experimenter has reached an erroneous conclusion concerning this factor. Now if



(a) Small distance between factor levels



(b) Aggressive spacing of factor levels

Figure 6-9 The impact of the choice of factor levels in an unreplicated design.

there is less variability in the response, the likelihood of an erroneous conclusion will be smaller. Another way to ensure that reliable effect estimates are obtained is to increase the distance between the low (−) and high (+) levels of the factor, as illustrated in Figure 6-9*b*. Notice that in this figure, the increased distance between the low and high factor levels results in a reasonable estimate of the true factor effect.

The single-replicate strategy is often used in screening experiments when there are relatively many factors under consideration. Because we can never be entirely certain in such cases that the experimental error is small, a good practice in these types of experiments is to spread out the factor levels aggressively. You might find it helpful to re-read the guidance on choosing factor levels in Chapter 1.

A single replicate of a 2^k design is sometimes called an **unreplicated factorial**. With only one replicate, there is no internal estimate of error (or "pure error"). One approach to the analysis of an unreplicated factorial is to assume that certain high-order interactions are negligible and combine their mean squares to estimate the error. This is an appeal to the **sparsity of effects principle**; that is, most systems are dominated by some of the main effects and low-order interactions, and most high-order interactions are negligible.

When analyzing data from unreplicated factorial designs, occasionally real high-order interactions occur. The use of an error mean square obtained by pooling high-order interactions is inappropriate in these cases. A method of analysis attributed to Daniel (1959) provides a simple way to overcome this problem. Daniel suggests examining a **normal probability plot** of the estimates of the effects. The effects that are negligible are normally distributed, with mean zero and variance σ^2 and will tend to fall along a straight line on this plot, whereas significant effects will have nonzero means and will not lie along the straight line. Thus the preliminary model will be specified to contain those effects that are apparently nonzero, based on the normal probability plot. The apparently negligible effects are combined as an estimate of error.

EXAMPLE 6-2

A Single Replicate of the 2^4 Design

A chemical product is produced in a pressure vessel. A factorial experiment is carried out in the pilot plant to study the factors thought to influence the filtration rate of this product. The four factors are temperature (A), pressure (B), concentration of formaldehyde (C), and stirring rate (D). Each factor is present at two levels. The design matrix and the response data obtained from a single replicate of the 2^4 experiment are shown in Table 6-10 and Figure 6-10. The 16 runs are made in random order. The process engineer is interested in maximizing the filtration rate. Current process conditions give filtration rates of around 75 gal/h. The process also currently uses the concentration of formaldehyde, factor C, at the high level. The engineer would like to reduce the formaldehyde concentration as much as possible but has been unable to do so because it always results in lower filtration rates.

We will begin the analysis of this data by constructing a normal probability plot of the effect estimates. The table of plus and minus signs for the contrast constants for the

Table 6-10 Pilot Plant Filtration Rate Experiment

Run Number	Factor				Run Label	Filtration Rate (gal/h)
	A	B	C	D		
1	−	−	−	−	(1)	45
2	+	−	−	−	a	71
3	−	+	−	−	b	48
4	+	+	−	−	ab	65
5	−	−	+	−	c	68
6	+	−	+	−	ac	60
7	−	+	+	−	bc	80
8	+	+	+	−	abc	65
9	−	−	−	+	d	43
10	+	−	−	+	ad	100
11	−	+	−	+	bd	45
12	+	+	−	+	abd	104
13	−	−	+	+	cd	75
14	+	−	+	+	acd	86
15	−	+	+	+	bcd	70
16	+	+	+	+	$abcd$	96

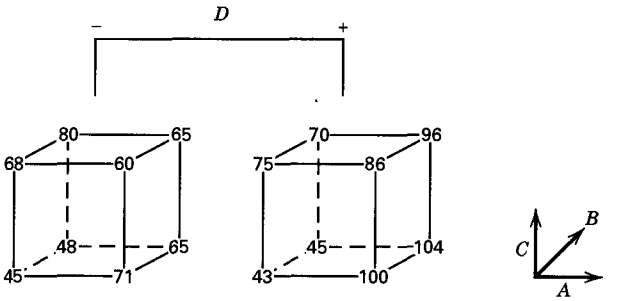


Figure 6-10 Data from the pilot plant filtration rate experiment for Example 6-2.

2^4 design are shown in Table 6-11 (page 248). From these contrasts, we may estimate the 15 factorial effects and the sums of squares shown in Table 6-12 (page 249).

The normal probability plot of these effects is shown in Figure 6-11 (page 249). All of the effects that lie along the line are negligible, whereas the large effects are far from the line. The important effects that emerge from this analysis are the main effects of A, C, and D and the AC and AD interactions.

The main effects of A, C, and D are plotted in Figure 6-12*a* (page 250). All three effects are positive, and if we considered only these main effects, we would run all three factors at the high level to maximize the filtration rate. However, it is always necessary to examine any interactions that are important. Remember that main effects do not have much meaning when they are involved in significant interactions.

The AC and AD interactions are plotted in Figure 6-12*b*. These interactions are the key to solving the problem. Note from the AC interaction that the temperature effect is very small when the concentration is at the high level and very large when the concentration is at the low level, with the best results obtained with low concentration and high temperature. The AD interaction indicates that stirring rate D has little effect at low temperature but a large positive effect at high temperature. Therefore, the best filtration rates would appear to be obtained when A and D are at the high level and C is at the low level. This would allow the reduction of the formaldehyde concentration to a lower level, another objective of the experimenter.

Design Projection

Another interpretation of the effects in Figure 6-11 is possible. Because B (pressure) is not significant and all interactions involving B are negligible, we may discard B from the experiment so that the design becomes a 2^3 factorial in A, C, and D with two replicates. This is easily seen from examining only columns A, C, and D in the design matrix shown in Table 6-10 and noting that those columns form two replicates of a 2^3 design. The analysis of variance for the data using this simplifying assumption is summarized in Table 6-13 (page 250). The conclusions that we would draw from this analysis are essentially unchanged from those of Example 6-2. Note that by projecting the single replicate of the 2^4 into a replicated 2^3, we now have both an estimate of the ACD interaction and an estimate of error based on what is sometimes called **hidden replication.**

Table 6-11 Contrast Constants for the 2^4 Design

	A	*B*	*AB*	*C*	*AC*	*BC*	*ABC*	*D*	*AD*	*BD*	*ABD*	*CD*	*ACD*	*BCD*	*ABCD*
(1)	−	−	+	−	+	+	−	−	+	+	−	+	−	−	+
a	+	−	−	−	−	+	+	−	−	+	+	+	+	−	−
b	−	+	−	−	+	−	+	−	+	−	+	+	−	+	−
ab	+	+	+	−	−	−	−	−	−	−	−	+	+	+	+
c	−	−	+	+	−	−	+	−	+	+	−	−	+	+	−
ac	+	−	−	+	+	−	−	−	−	+	+	−	−	+	+
bc	−	+	−	+	−	+	−	−	+	−	+	−	+	−	+
abc	+	+	+	+	+	+	+	−	−	−	−	−	−	−	−
d	−	−	+	−	+	+	−	+	−	−	+	−	+	+	−
ad	+	−	−	−	−	+	+	+	+	−	−	−	−	+	+
bd	−	+	−	−	+	−	+	+	−	+	−	−	+	−	+
abd	+	+	+	−	−	−	−	+	+	+	+	−	−	−	−
cd	−	−	+	+	−	−	+	+	−	−	+	+	−	−	+
acd	+	−	−	+	+	−	−	+	+	−	−	+	+	−	−
bcd	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−
abcd	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+

Table 6-12 Factor Effect Estimates and Sums of Squares for the 2^4 Factorial in Example 6-2

Model Term	Effect Estimate	Sum of Squares	Percent Contribution
A	21.625	1870.56	32.6397
B	3.125	39.0625	0.681608
C	9.875	390.062	6.80626
D	14.625	855.563	14.9288
AB	0.125	0.0625	0.00109057
AC	−18.125	1314.06	22.9293
AD	16.625	1105.56	19.2911
BC	2.375	22.5625	0.393696
BD	−0.375	0.5625	0.00981515
CD	−1.125	5.0625	0.0883363
ABC	1.875	14.0625	0.245379
ABD	4.125	68.0625	1.18763
ACD	−1.625	10.5625	0.184307
BCD	−2.625	27.5625	0.480942
ABCD	1.375	7.5625	0.131959

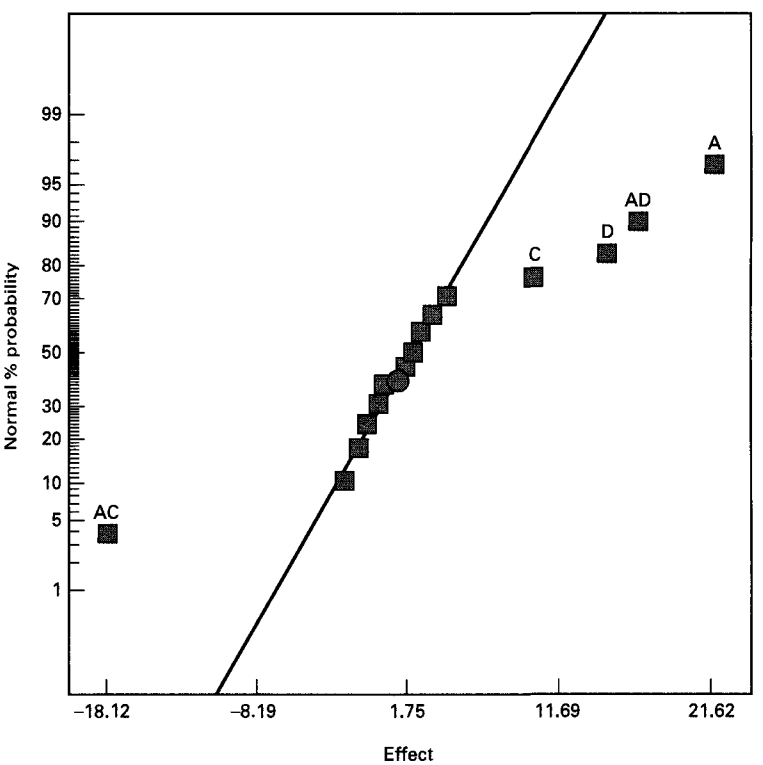
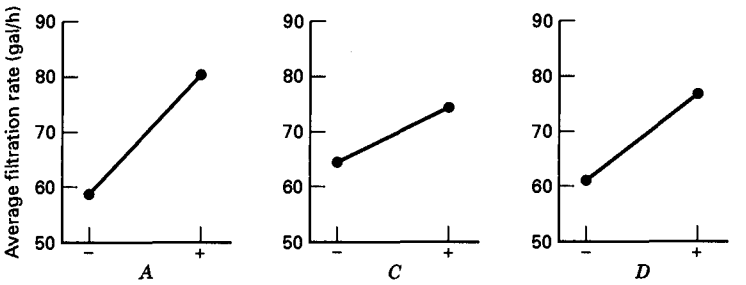
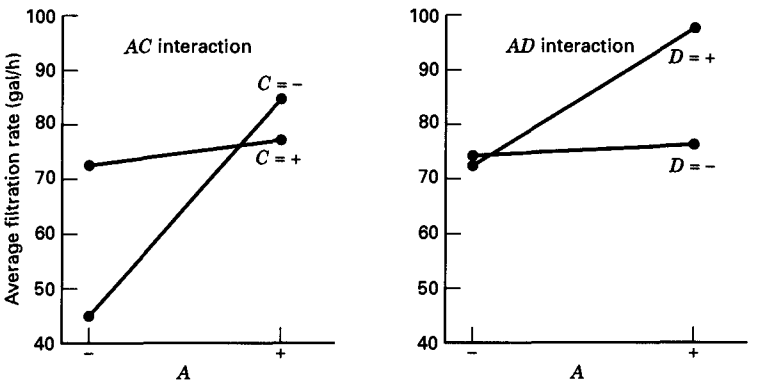


Figure 6-11 Normal probability plot of the effects for the 2^4 factorial in Example 6-2.



(a) Main effect plots



(b) Interaction plots

Figure 6-12 Main effect and interaction plots for Example 6-2.

Table 6-13 Analysis of Variance for the Pilot Plant Filtration Rate Experiment in A, C, and D

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
A	1870.56	1	1870.56	83.36	<0.0001
C	390.06	1	390.06	17.38	<0.0001
D	855.56	1	855.56	38.13	<0.0001
AC	1314.06	1	1314.06	58.56	<0.0001
AD	1105.56	1	1105.56	49.27	<0.0001
CD	5.06	1	5.06	<1	
ACD	10.56	1	10.56	<1	
Error	179.52	8	22.44		
Total	5730.94	15			

The concept of projecting an unreplicated factorial into a replicated factorial in fewer factors is very useful. In general, if we have a single replicate of 2^k design, and if h ($h < k$) factors are negligible and can be dropped, then the original data correspond to a full two-level factorial in the remaining $k - h$ factors with 2^h replicates.

Diagnostic Checking

The usual diagnostic checks should be applied to the residuals of a 2^k design. Our analysis indicates that the only significant effects are $A = 21.625$, $C = 9.875$, $D = 14.625$, $AC = -18.125$, and $AD = 16.625$. If this is true, the estimated filtration rates are given by

$$\hat{y} = 70.06 + \left(\frac{21.625}{2}\right)x_1 + \left(\frac{9.875}{2}\right)x_3 + \left(\frac{14.625}{2}\right)x_4 - \left(\frac{18.125}{2}\right)x_1x_3 + \left(\frac{16.625}{2}\right)x_1x_4$$

where 70.06 is the average response and the coded variables x_1, x_3, x_4 take on values between -1 and $+1$. The predicted filtration rate at run (1) is

$$\hat{y} = 70.06 + \left(\frac{21.625}{2}\right)(-1) + \left(\frac{9.875}{2}\right)(-1) + \left(\frac{14.625}{2}\right)(-1) - \left(\frac{18.125}{2}\right)(-1)(-1) + \left(\frac{16.625}{2}\right)(-1)(-1)$$

$$= 46.22$$

Because the observed value is 45, the residual is $e = y - \hat{y} = 45 - 46.22 = -1.22$. The values of y, $\hat{y}$, and $e = y - \hat{y}$ for all 16 observations follow.

	y	$\hat{y}$	$e = y - \hat{y}$
(1)	45	46.22	−1.22
a	71	69.39	1.61
b	48	46.22	1.78
ab	65	69.39	−4.39
c	68	74.23	−6.23
ac	60	61.14	−1.14
bc	80	74.23	5.77
abc	65	61.14	3.86
d	43	44.22	−1.22
ad	100	100.65	−0.65
bd	45	44.22	0.78
abd	104	100.65	3.35
cd	75	72.23	2.77
acd	86	92.40	−6.40
bcd	70	72.23	−2.23
abcd	96	92.40	3.60

A normal probability plot of the residuals is shown in Figure 6-13 on the next page. The points on this plot lie reasonably close to a straight line, lending support to our conclusion

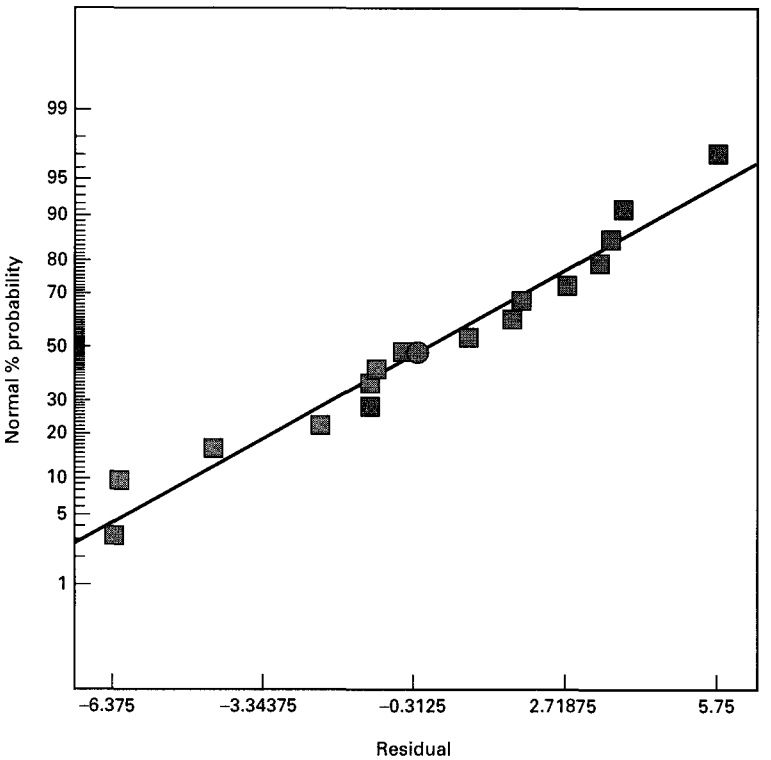


Figure 6-13 Normal probability plot of residuals for Example 6-2.

that A, C, D, AC, and AD are the only significant effects and that the underlying assumptions of the analysis are satisfied.

The Response Surface

We used the interaction plots in Figure 6-12 to provide a practical interpretation of the results of this experiment. Sometimes we find it helpful to use the response surface for this purpose. The response surface is generated by the regression model

$$\hat{y} = 70.06 + \left(\frac{21.625}{2}\right) x_1 + \left(\frac{9.875}{2}\right) x_3 + \left(\frac{14.625}{2}\right) x_4 - \left(\frac{18.125}{2}\right) x_1x_3 + \left(\frac{16.625}{2}\right) x_1x_4$$

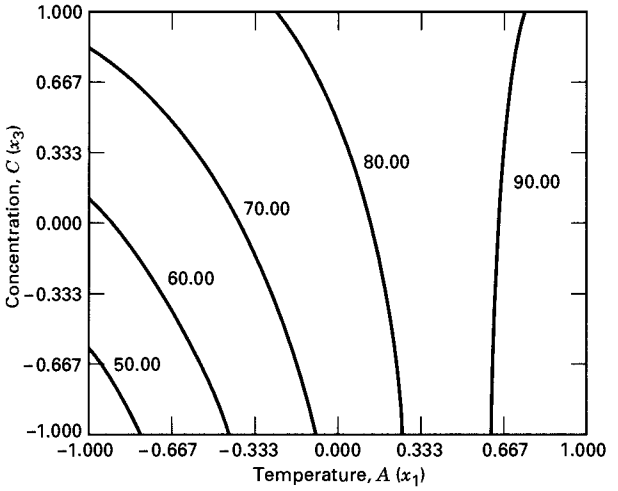
Figure 6-14*a* shows the response surface contour plot when stirring rate is at the high level (i.e., $x_4 = 1$). The contours are generated from the above model with $x_4 = 1$, or

$$\hat{y} = 77.3725 + \left(\frac{38.25}{2}\right) x_1 + \left(\frac{9.875}{2}\right) x_3 - \left(\frac{18.125}{2}\right) x_1x_3$$

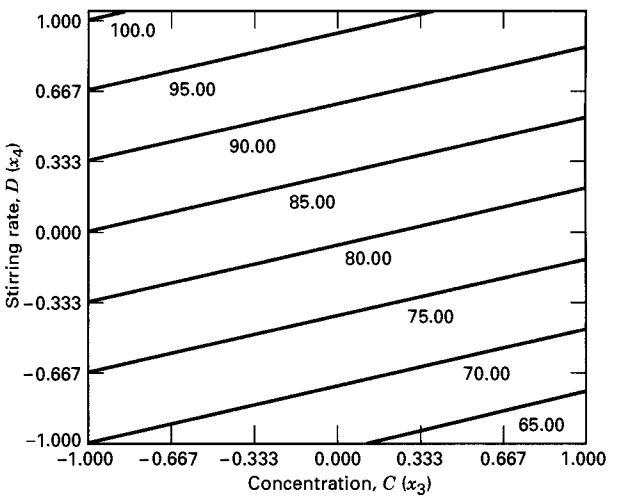
Notice that the contours are curved lines because the model contains an interaction term.

Figure 6-14*b* is the response surface contour plot when temperature is at the high level (i.e., $x_1 = 1$). When we put $x_1 = 1$ in the regression model we obtain

$$\hat{y} = 80.8725 - \left(\frac{8.25}{2}\right) x_3 + \left(\frac{31.25}{2}\right) x_4$$



(*a*) Contour plot with stirring rate (D), $x_4 = 1$



(*b*) Contour plot with with temperature (A), $x_1 = 1$

Figure 6-14 Contour plots of filtration rate, Example 6-2.

These contours are parallel straight lines because the model contains only the main effects of factors C (x_3) and D (x_4).

Both contour plots indicate that if we want to maximize the filtration rate, variables A (x_1) and D (x_4) should be at the high level and that the process is relatively robust to concentration C. We obtained similar conclusions from the interaction graphs.

The Half-Normal Plot of Effects

An alternative to the normal probability plot of the factor effects is the **half-normal plot**. This is a plot of the absolute value of the effect estimates against their cumulative normal probabilities. Figure 6-15 (page 254) presents the half-normal plot of the effects for Example 6-2. The straight line on the half-normal plot always passes through the origin and should also pass close to the fiftieth percentile data value. Many analysts feel that the half-normal plot is easier to interpret, particularly when there are only a few effect

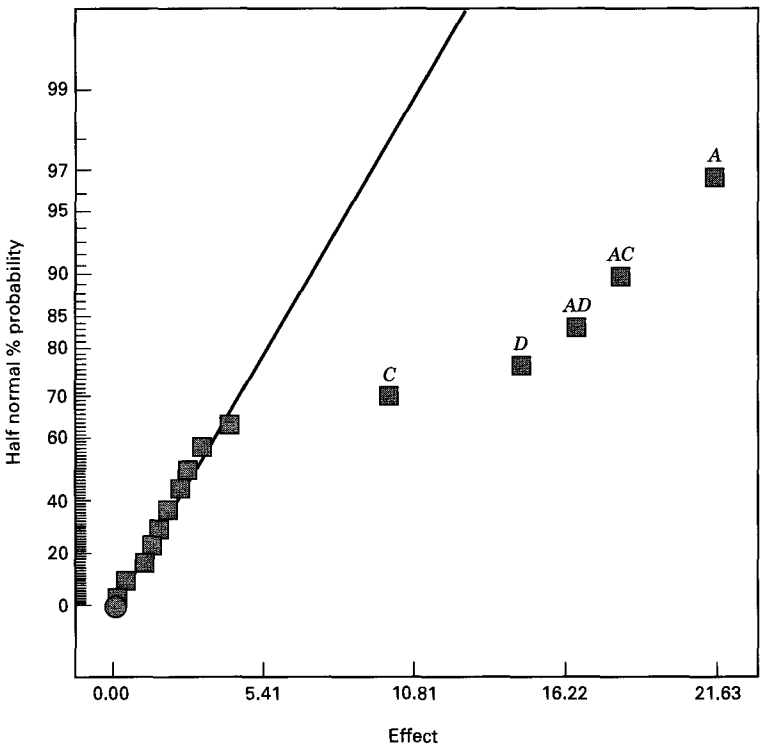


Figure 6-15 Half-normal plot of the factor effects from Example 6-2.

estimates such as when the experimenter has used an eight-run design. Some software packages will construct both plots.

Other Methods for Analyzing Unreplicated Factorials

The standard analysis procedure for an unreplicated two-level factorial design is the normal (or half-normal) plot of the estimated factor effects. However, unreplicated designs are so widely used in practice that many formal analysis procedures have been proposed to overcome the subjectivity of the normal probability plot. Hamada and Balakrishnan (1998) compared some of these methods. They found that the method proposed by Lenth (1989) has good power to detect significant effects. It is also easy to implement, and as a result, it is beginning to appear in some software packages for analyzing data from unreplicated factorials. We give a brief description of Lenth's method.

Suppose that we have m contrasts of interest, say $c_1, c_2, \ldots, c_m$. If the design is an unreplicated 2^k factorial design, these contrasts correspond to the $m = 2^k - 1$ factor effect estimates. The basis of Lenth's method is to estimate the variance of a contrast from the smallest (in absolute value) contrast estimates. Let

$$s_0 = 1.5 \times \text{median}(|c_j|)$$

and

$$PSE = 1.5 \times \text{median}(|c_j| : |c_j| < 2.5s_0)$$

PSE is called the "pseudo standard error," and Lenth shows that it is a reasonable estimator of the contrast variance when there are not many active (significant) effects. The *PSE* is used to judge the significance of contrasts. An individual contrast can be compared to the **margin of error**

$$ME = t_{0.025,d} \times PSE$$

where the degrees of freedom are defined as $d = m/3$. For inference on a group of contrasts Lenth suggests using the **simultaneous margin of error**

$$SME = t_{\gamma,d} \times PSE$$

where the percentage point of the t distribution used is $\gamma = 1 - (1 + 0.95^{1/m})/2$.

To illustrate Lenth's method, consider the 2^4 experiment in Example 6-2. The calculations result in $s_0 = 1.5 \times |-2.625| = 3.9375$ and $2.5 \times 3.9375 = 9.84375$, so

$$\begin{aligned} PSE &= 1.5 \times |1.75| = 2.625 \\ ME &= 2.571 \times 2.625 = 6.75 \\ SME &= 5.219 \times 2.625 = 13.70 \end{aligned}$$

Now consider the effect estimates in Table 6-12. The *SME* criterion would indicate that the four largest effects (in magnitude) are significant, because their effect estimates exceed *SME*. The main effect of *C* is significant according to the *ME* criterion, but not with respect to *SME*. However, because the *AC* interaction is clearly important, we would probably include *C* in the list of significant effects. Notice that in this example, Lenth's method has produced the same answer that we obtained previously from examination of the normal probability plot of effects.

Several authors [see Hamada and Balakrishnan (1998), Loughin (1998), Loughin and Noble (1997), and Larntz and Whitcomb (1998)] have observed that Lenth's method fails to control type I error rates, and that simulation methods can be used to calibrate his procedure. Larntz and Whitcomb (1998) suggest replacing the original *ME* and *SME* multipliers with **adjusted multipliers** as follows:

Number of Contrasts	7	15	31
Original *ME*	3.764	2.571	2.218
Adjusted *ME*	2.295	2.140	2.082
Original *SME*	9.008	5.219	4.218
Adjusted *SME*	4.891	4.163	4.030

These are in close agreement with the results in Ye and Hamada (2000).

In general, the Lenth method is a clever and useful procedure. However, we recommend using it as a **supplement** to the usual normal probability plot of effects, not as a replacement for it.

Bisgaard (1998–1999) has provided a nice graphical technique, called a **conditional inference chart**, to assist in interpreting the normal probability plot. The purpose of the graph is to help the experimenter in judging significant effects. This would be relatively easy if the standard deviation σ were known, or if it could be estimated from the data. In unreplicated designs, there is no internal estimate of σ, so the conditional inference chart is designed to help the experimenter evaluate effect magnitude for a *range* of

standard deviation values. Bisgaard bases the graph on the result that the standard error of an effect in a two-level design with N runs (for an unreplicated factorial, $N = 2^k$) is

$$\frac{2\sigma}{\sqrt{N}}$$

where σ is the standard deviation of an individual observation. Then ± 2 times the standard error of an effect is

$$\pm\frac{4\sigma}{\sqrt{N}}$$

Once the effects are estimated, plot a graph as shown in Figure 6-16, with the effect estimates plotted along the vertical, or y-axis. In this figure, we have used the effect estimates from Example 6-2.The horizontal, or x-axis, of Figure 6-16 is a standard deviation (σ) scale. The two lines are at

$$y = +\frac{4\sigma}{\sqrt{N}} \quad \text{and} \quad y = -\frac{4\sigma}{\sqrt{N}}$$

In our example, $N = 16$, so the lines are at $y = +\sigma$ and $y = -\sigma$. Thus, for any given value of the standard deviation σ we can read off the distance between these two lines as an approximate 95 percent confidence interval on the negligible effects.

In Figure 6-16, we observe that if the experimenter thinks that the standard deviation is between 4 and 8, then factors A, C, D, and the AC and AD interactions are significant. If he or she thinks that the standard deviation is as large as 10, factor C may not be

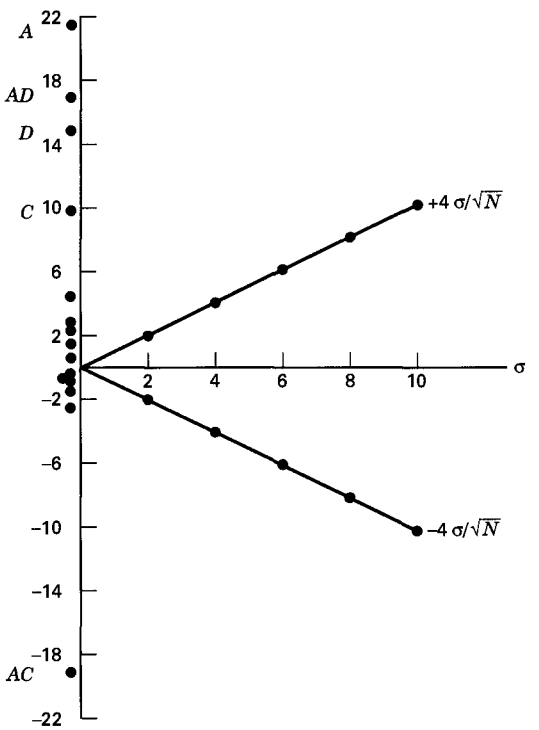


Figure 6-16 A conditional inference chart for Example 6-2.

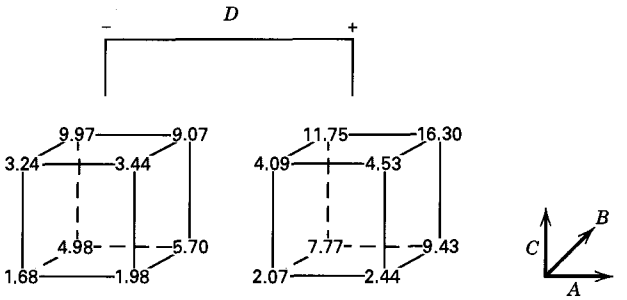


Figure 6-17 Data from the drilling experiment of Example 6-3.

significant. That is, for any given assumption about the magnitude of σ, the experimenter can construct a "yardstick" for judging the approximate significance of effects. The chart can also be used in reverse. For example, suppose that we were uncertain about whether factor C is significant. The experimenter could then ask whether it is reasonable to expect that σ could be as large as 10 or more. If it is unlikely that σ is as large as 10, then we can conclude that C is significant.

We now present three instructive examples of unreplicated 2^k factorial designs.

EXAMPLE 6-3

Data Transformation in a Factorial Design

Daniel (1976) describes a 2^4 factorial design used to study the advance rate of a drill as a function of four factors: drill load (A), flow rate (B), rotational speed (C), and the type of drilling mud used (D). The data from the experiment are shown in Figure 6-17.

The normal probability plot of the effect estimates from this experiment is shown in Figure 6-18. Based on this plot, factors B, C, and D along with the BC and BD interactions

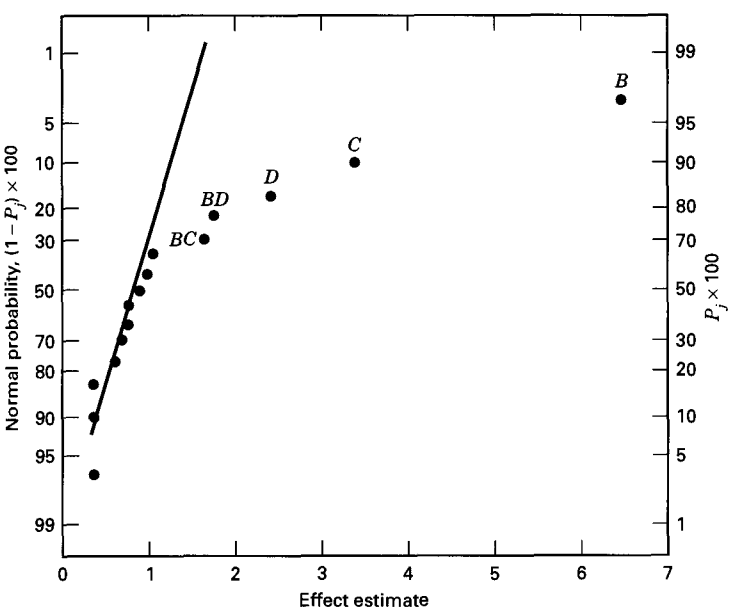


Figure 6-18 Normal probability plot of effects for Example 6-3.

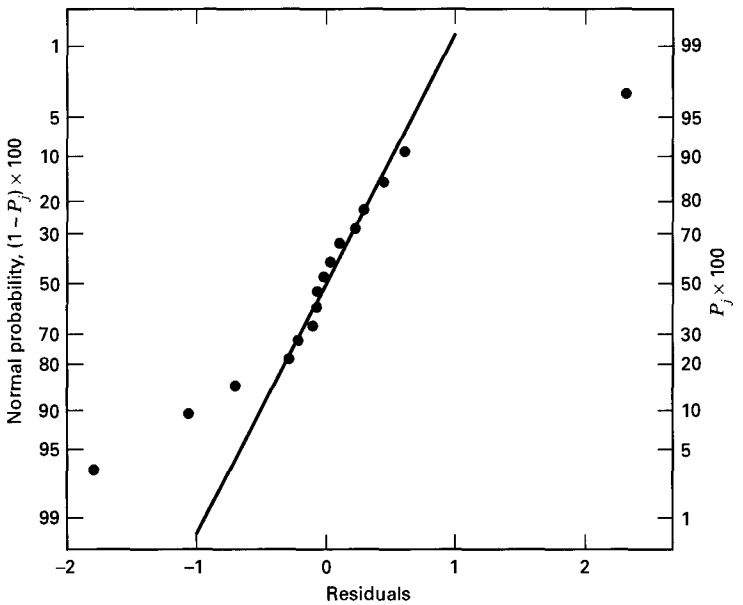


Figure 6-19 Normal probability plot of residuals for Example 6-3.

require interpretation. Figure 6-19 is the normal probability plot of the residuals and Figure 6-20 is the plot of the residuals versus the predicted advance rate from the model containing the identified factors. There are clearly problems with normality and equality of variance. A data transformation is often used to deal with such problems. Because the response variable is a rate, the log transformation seems a reasonable candidate.

Figure 6-21 presents a normal probability plot of the effect estimates following the

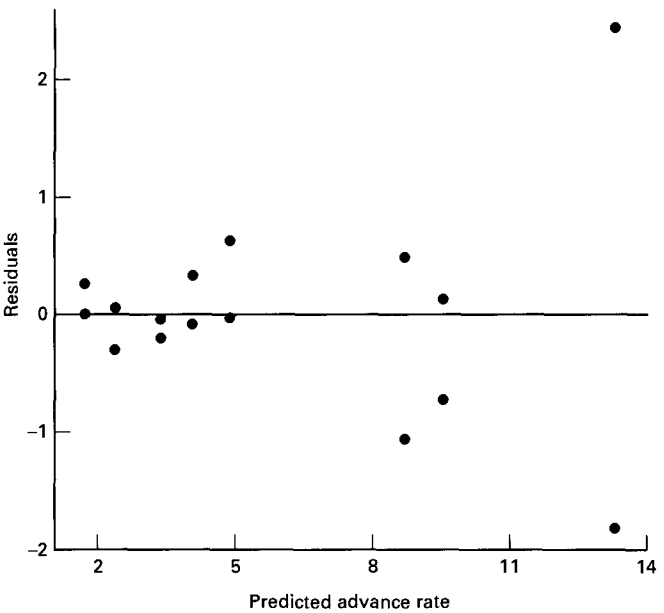


Figure 6-20 Plot of residuals versus predicted rate for Example 6-3.

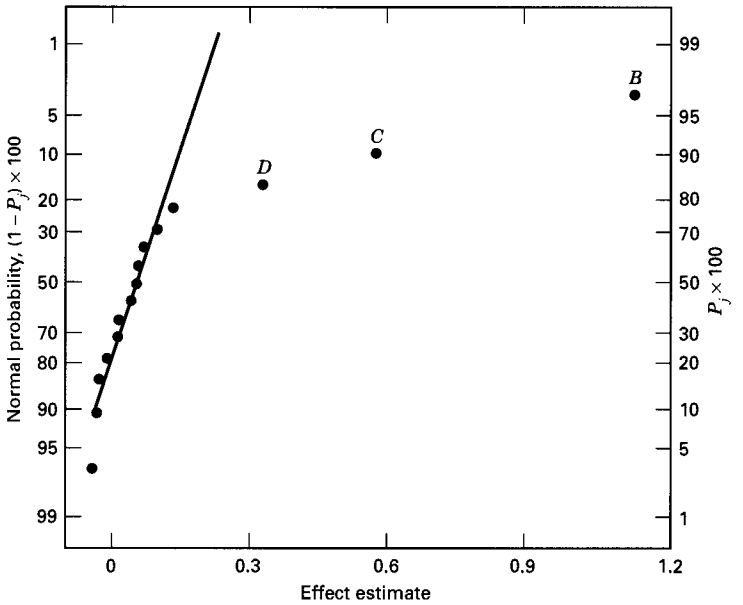


Figure 6-21 Normal probability plot of effects for Example 6-3 following log transformation.

transformation $y^* = \ln y$. Notice that a much simpler interpretation now seems possible, because only factors B, C, and D are active. That is, expressing the data in the correct metric has simplified its structure to the point that the two interactions are no longer required in the explanatory model.

Figures 6-22 and 6-23 present, respectively, a normal probability plot of the residuals

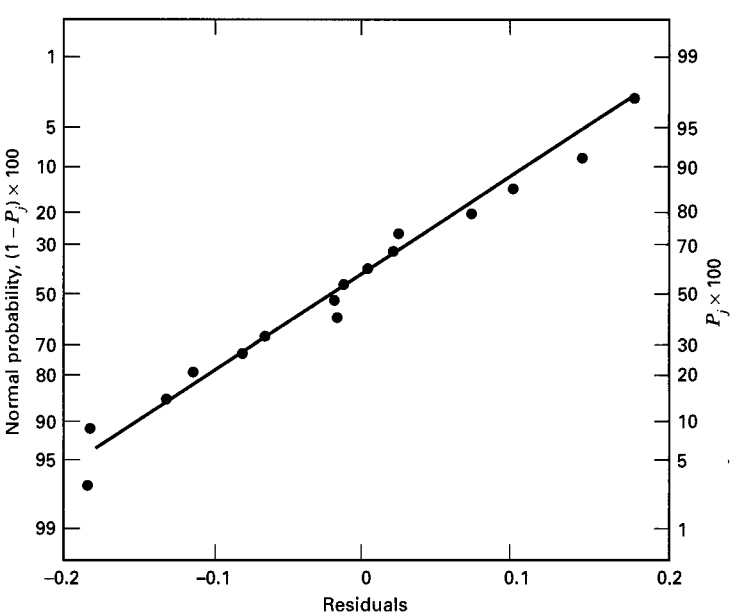


Figure 6-22 Normal probability plot of residuals for Example 6-3 following log transformation.

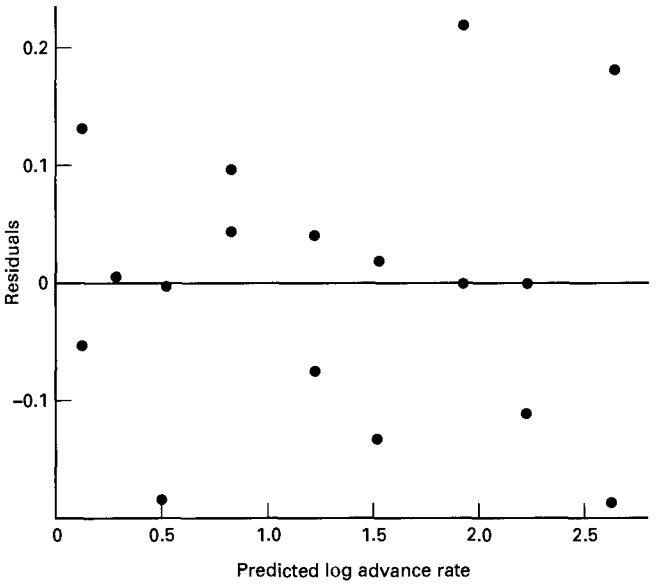


Figure 6-23 Plot of residuals versus predicted rate for Example 6-3 following log transformation.

and a plot of the residuals versus the predicted advance rate for the model in the log scale containing B, C, and D. These plots are now satisfactory. We conclude that the model for $y^* = \ln y$ requires only factors B, C, and D for adequate interpretation. The analysis of variance for this model is summarized in Table 6-14. The model sum of squares is

$$\begin{aligned} SS_{\text{Model}} &= SS_B + SS_C + SS_D \\ &= 5.345 + 1.339 + 0.431 \\ &= 7.115 \end{aligned}$$

and $R^2 = SS_{\text{Model}}/SS_T = 7.115/7.288 = 0.98$, so the model explains about 98 percent of the variability in the drill advance rate.

EXAMPLE 6-4

Location and Dispersion Effects in an Unreplicated Factorial

A 2^4 design was run in a manufacturing process producing interior side-wall and window panels for commercial aircraft. The panels are formed in a press, and under present

Table 6-14 Analysis of Variance for Example 6-3 Following the Log Transformation

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
B (Flow)	5.345	1	5.345	381.79	<0.0001
C (Speed)	1.339	1	1.339	95.64	<0.0001
D (Mud)	0.431	1	0.431	30.79	<0.0001
Error	0.173	12	0.014		
Total	7.288	15			

Factors	Low (−)	High (+)
A = Temperature (°F)	295	325
B = Clamp time (min)	7	9
C = Resin flow	10	20
D = Closing time (s)	15	30

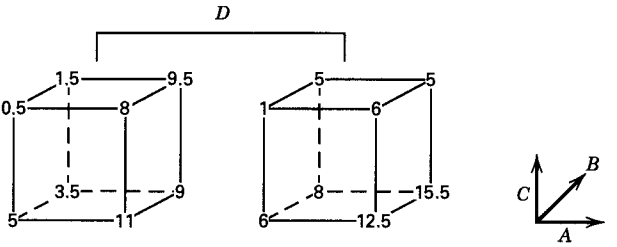


Figure 6-24 Data for the panel process experiment of Example 6-4.

conditions the average number of defects per panel in a press load is much too high. (The current process average is 5.5 defects per panel.) Four factors are investigated using a single replicate of a 2^4 design, with each replicate corresponding to a single press load. The factors are temperature (A), clamp time (B), resin flow (C), and press closing time (D). The data for this experiment are shown in Figure 6-24.

A normal probability plot of the factor effects is shown in Figure 6-25. Clearly the two largest effects are $A = 5.75$ and $C = -4.25$. No other factor effects appear to be large, and A and C explain about 77 percent of the total variability, so we conclude that lower temperature (A) and higher resin flow (C) would reduce the incidence of panel defects.

Careful residual analysis is an important aspect of any experiment. A normal probability plot of the residuals showed no anomalies, but when the experimenter plotted the residuals versus each of the factors A through D, the plot of residuals versus B (clamp

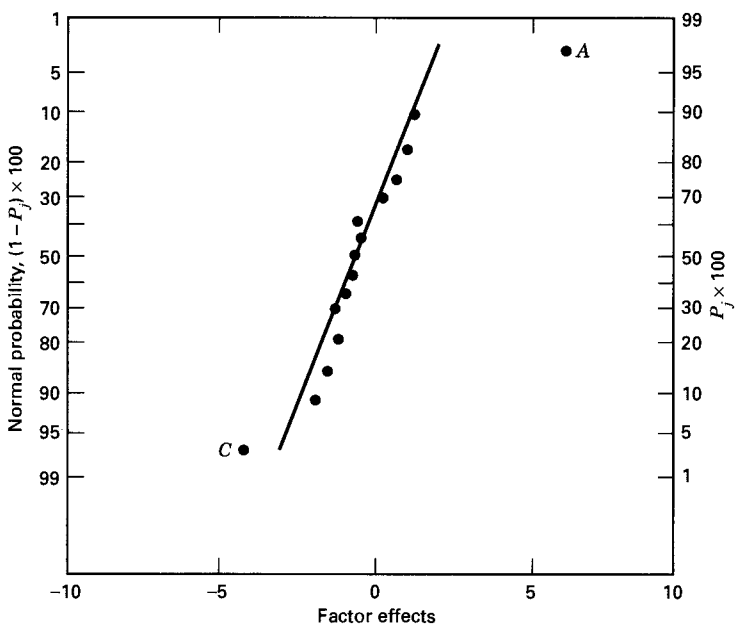


Figure 6-25 Normal probability plot of the factor effects for the panel process experiment of Example 6-4.

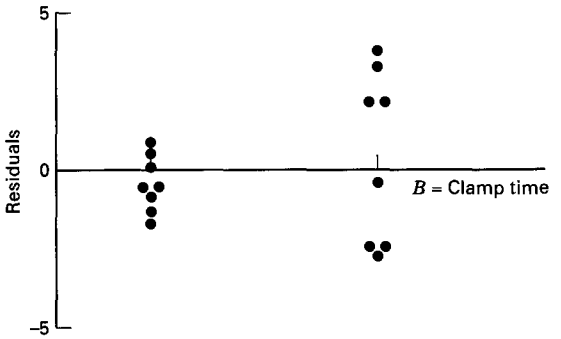


Figure 6-26 Plot of residuals versus clamp time for Example 6-4.

time) presented the pattern in Figure 6-26. This factor, which is unimportant insofar as the average number of defects per panel is concerned, is very important in its effect on process variability, with the lower clamp time resulting in less variability in the average number of defects per panel in a press load.

The dispersion effect of clamp time is also very evident from the **cube plot** in Figure 6-27, which plots the average number of defects per panel and the range of the number of defects at each point in the cube defined by factors A, B, and C. The average range when B is at the high level (the back face of the cube in Figure 6-27) is $\bar{R}_{B^+} = 4.75$, and when B is at the low level it is $\bar{R}_{B^-} = 1.25$.

As a result of this experiment, the engineer decided to run the process at low temperature and high resin flow to reduce the average number of defects, at low clamp time to reduce the variability in the number of defects per panel, and at low press closing time (which had no effect on either location or dispersion). The new set of operating conditions resulted in a new process average of less than one defect per panel.

The residuals from a 2^k design provide much information about the problem under study. Because residuals can be thought of as observed values of the noise or error, they often give insight into process variability. We can systematically examine the residuals from an unreplicated 2^k design to provide information about process variability.

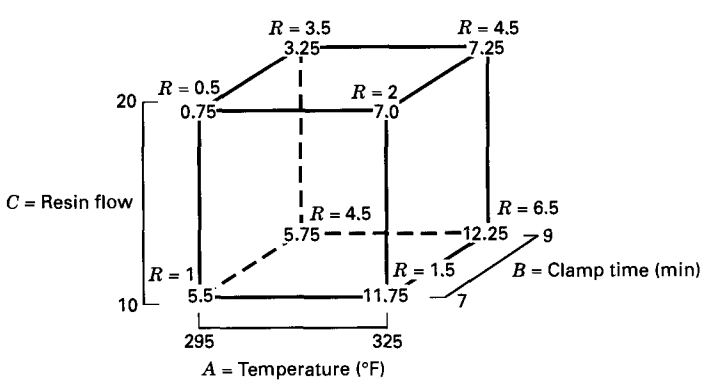


Figure 6-27 Cube plot of temperature, clamp time, and resin flow for Example 6-4.

Table 6-15 Calculation of Dispersion Effects for Example 6-4

Run	*A*	*B*	*AB*	*C*	*AC*	*BC*	*ABC*	*D*	*AD*	*BD*	*ABD*	*CD*	*ACD*	*BCD*	*ABCD*	Residual
1	−	−	+	−	+	+	−	−	+	+	−	+	−	−	+	−0.94
2	+	−	−	−	−	+	+	−	−	+	+	+	+	−	−	−0.69
3	−	+	−	−	+	−	+	−	+	−	+	+	−	+	−	−2.44
4	+	+	+	−	−	−	−	−	−	−	−	+	+	+	+	−2.69
5	−	−	+	+	−	−	+	−	+	+	−	−	+	+	−	−1.19
6	+	−	−	+	+	−	−	−	−	+	+	−	−	+	+	0.56
7	−	+	−	+	−	+	−	−	+	−	+	−	+	−	+	−0.19
8	+	+	+	+	+	+	+	−	−	−	−	−	−	−	−	2.06
9	−	−	+	−	+	+	−	+	−	−	+	−	+	+	−	0.06
10	+	−	−	−	−	+	+	+	+	−	−	−	−	+	+	0.81
11	−	+	−	−	+	−	+	+	−	+	−	−	+	−	+	2.06
12	+	+	+	−	−	−	−	+	+	+	+	−	−	−	−	3.81
13	−	−	+	+	−	−	+	+	−	−	+	+	−	−	+	−0.69
14	+	−	−	+	+	−	−	+	+	−	−	+	+	−	−	−1.44
15	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	3.31
16	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	−2.44
$S(i^+)$	2.25	2.72	2.21	1.91	1.81	1.80	1.80	2.24	2.05	2.28	1.97	1.93	1.52	2.09	1.61	
$S(i^-)$	1.85	0.83	1.86	2.20	2.24	2.26	2.24	1.55	1.93	1.61	2.11	1.58	2.16	1.89	2.33	
F_i^*	0.39	2.37	0.34	−0.28	−0.43	−0.46	−0.44	0.74	0.12	0.70	−0.14	0.40	−0.70	0.28	−0.74	

Consider the residual plot in Figure 6-26. The standard deviation of the eight residuals where B is at the low level is $S(B^-) = 0.83$, and the standard deviation of the eight residuals where B is at the high level is $S(B^+) = 2.72$. The statistic

$$F_B^* = \ln \frac{S^2(B^+)}{S^2(B^-)} \tag{6-24}$$

has an approximate normal distribution if the two variances $\sigma^2(B^+)$ and $\sigma^2(B^-)$ are equal. To illustrate the calculations, the value of F_B^* is

$$\begin{aligned} F_B^* &= \ln \frac{S^2(B^+)}{S^2(B^-)} \\ &= \ln \frac{(2.72)^2}{(0.83)^2} \\ &= 2.37 \end{aligned}$$

Table 6-15 (on the previous page) presents the complete set of contrasts for the 2^4 design along with the residuals for each run from the panel process experiment in Example 6-4. Each column in this table contains an equal number of plus and minus signs, and we can calculate the standard deviation of the residuals for each group of signs in each column, say $S(i^+)$ and $S(i^-)$, $i = 1, 2, \ldots, 15$. Then

$$F_i^* = \ln \frac{S^2(i^+)}{S^2(i^-)} \qquad i = 1, 2, \ldots, 15 \tag{6-25}$$

is a statistic that can be used to assess the magnitude of the **dispersion effects** in the experiment. If the variance of the residuals for the runs where factor i is positive equals the variance of the residuals for the runs where factor i is negative, then F_i^* has an approximate normal distribution. The values of F_i^* are shown below each column in Table 6-15.

Figure 6-28 is a normal probability plot of the dispersion effects F_i^*. Clearly, B is an important factor with respect to process dispersion. For more discussion of this pro-

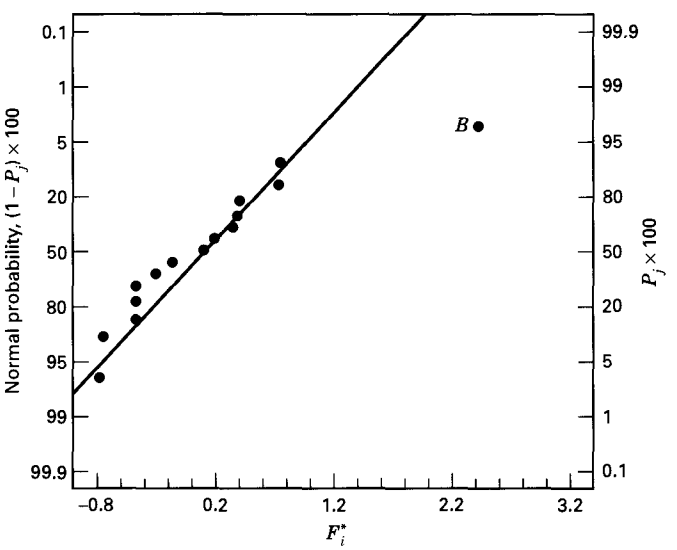


Figure 6-28 Normal probability plot of the dispersion effects F_i^* for Example 6-4.

cedure, see Box and Meyer (1986) and Myers and Montgomery (1995). Also, in order for the model residuals to properly convey information about dispersion effects, the **location model** must be correctly specified. Refer to the supplemental text material for this chapter for more details and an example.

EXAMPLE 6-5

Duplicate Measurements on the Response

A team of engineers at a semiconductor manufacturer ran a 2^4 factorial design in a vertical oxidation furnace. Four wafers are "stacked" in the furnace, and the response variable of interest is the oxide thickness on the wafers. The four design factors are temperature (A), time (B), pressure (C), and gas flow (D). The experiment is conducted by loading four wafers into the furnace, setting the process variables to the test conditions required by the experimental design, processing the wafers, and then measuring the oxide thickness on all four wafers. Table 6-16 presents the design and the resulting thickness measurements. In this table, the four columns labeled "Thickness" contain the oxide thickness measurements on each individual wafer, and the last two columns contain the sample average and sample variance of the thickness measurements on the four wafers in each run.

The proper analysis of this experiment is to consider the individual wafer thickness measurements as **duplicate measurements**, and not as replicates. If they were really replicates, each wafer would have been processed individually on a single run of the furnace. However, because all four wafers were processed together, they received the treatment factors (that is, the levels of the design variables) *simultaneously*, so there is much less variability in the individual wafer thickness measurements than would have been observed if each wafer was a replicate. Therefore, the **average** of the thickness measurements is the correct response variable to initially consider.

Table 6-17 (page 266) presents the effect estimates for this experiment, using the average oxide thickness $\bar{y}$ as the response variable. Note that factors A and B and the AB interaction have large effects that together account for nearly 90 percent of the variability

Table 6-16 The Oxide Thickness Experiment

Standard Order	Run Order	A	B	C	D	Thickness				$\bar{y}$	s^2
1	10	−1	−1	−1	−1	378	376	379	379	378	2
2	7	1	−1	−1	−1	415	416	416	417	416	0.67
3	3	−1	1	−1	−1	380	379	382	383	381	3.33
4	9	1	1	−1	−1	450	446	449	447	448	3.33
5	6	−1	−1	1	−1	375	371	373	369	372	6.67
6	2	1	−1	1	−1	391	390	388	391	390	2
7	5	−1	1	1	−1	384	385	386	385	385	0.67
8	4	1	1	1	−1	426	433	430	431	430	8.67
9	12	−1	−1	−1	1	381	381	375	383	380	12.00
10	16	1	−1	−1	1	416	420	412	412	415	14.67
11	8	−1	1	−1	1	371	372	371	370	371	0.67
12	1	1	1	−1	1	445	448	443	448	446	6
13	14	−1	−1	1	1	377	377	379	379	378	1.33
14	15	1	−1	1	1	391	391	386	400	392	34
15	11	−1	1	1	1	375	376	376	377	376	0.67
16	13	1	1	1	1	430	430	428	428	429	1.33

Table 6-17 Effect Estimates for Example 6-5, Response Variable Is Average Oxide Thickness

Model Term	Effect Estimate	Sum of Squares	Percent Contribution
A	43.125	7439.06	67.9339
B	18.125	1314.06	12.0001
C	−10.375	430.562	3.93192
D	−1.625	10.5625	0.0964573
AB	16.875	1139.06	10.402
AC	−10.625	451.563	4.12369
AD	1.125	5.0625	0.046231
BC	3.875	60.0625	0.548494
BD	−3.875	60.0625	0.548494
CD	1.125	5.0625	0.046231
ABC	−0.375	0.5625	0.00513678
ABD	2.875	33.0625	0.301929
ACD	−0.125	0.0625	0.000570753
BCD	−0.625	1.5625	0.0142688
ABCD	0.125	0.0625	0.000570753

in average oxide thickness. Figure 6-29 is a normal probability plot of the effects. From examination of this display, we would conclude that factors *A*, *B*, and *C* and the *AB* and *AC* interactions are important. The analysis of variance display for this model is shown in Table 6-18.

The model for predicting average oxide thickness is

$$\hat{y} = 399.19 + 21.56x_1 + 9.06x_2 - 5.19x_3 + 8.44x_1x_2 - 5.31x_1x_3$$

The residual analysis of this model is satisfactory.

The experimenters are interested in obtaining an average oxide thickness of 400 Å, and product specifications require that the thickness must lie between 390 and 410 Å. Figure 6-30 (page 268) presents two contour plots of average thickness, one with factor *C* (or x_3), pressure, at the low level (that is, $x_3 = -1$) and the other with *C* (or x_3) at the high level (that is, $x_3 = +1$). From examining these contour plots, it is obvious that there are many combinations of time and temperature (factors *A* and *B*) that will produce acceptable results. However, if pressure is held constant at the low level, the operating "window" is shifted toward the left, or lower, end of the time axis, indicating that lower cycle times will be required to achieve the desired oxide thickness.

It is interesting to observe the results that would be obtained if we **incorrectly** consider the individual wafer oxide thickness measurements as replicates. Table 6-19 (page 269) presents a full model analysis of variance based on treating the experiment as a replicated 2^4 factorial. Notice that there are many significant factors in this analysis, suggesting a much more complex model than we found when using the average oxide thickness as the response. The reason for this is that the estimate of the error variance in Table 6-19 is too small ($\hat{\sigma}^2 = 6.12$). The residual mean square in Table 6-19 reflects the variability between wafers *within* a run and variability *between* runs. The estimate of error obtained from Table 6-18 is much larger, $\hat{\sigma}^2 = 17.61$, and it is primarily a measure of the between-run variability. This is the best estimate of error to use in judging the significance of process variables that are changed from run to run.

A logical question to ask is: What harm results from identifying too many factors as

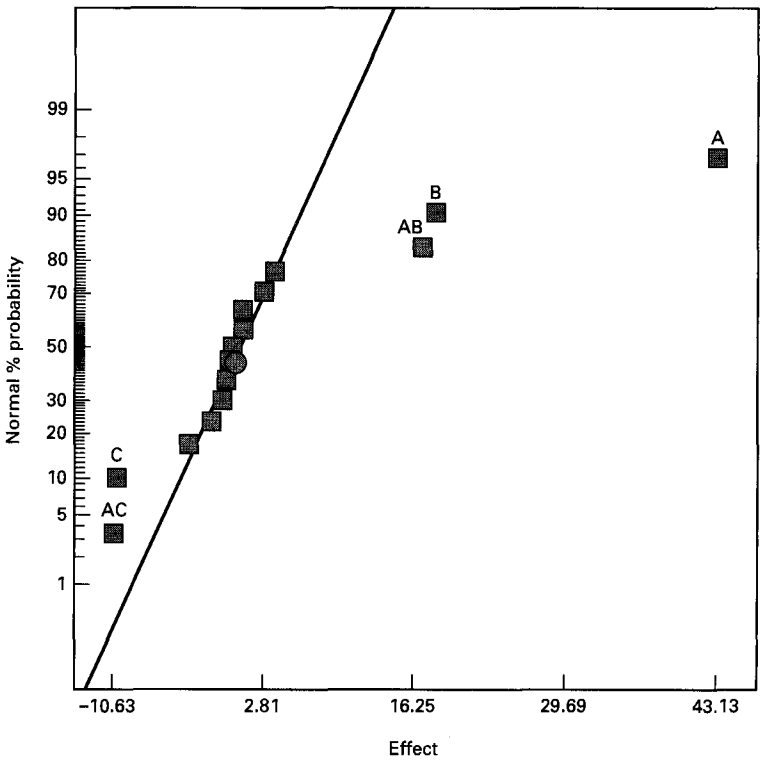


Figure 6-29 Normal probability plot of the effects for the average oxide thickness response, Example 6-5.

Table 6-18 Analysis of Variance (From Design-Expert) for the Average Oxide Thickness Response, Example 6-5

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	10774.31	5	2154.86	122.35	<0.000
A	*7439.06*	*1*	*7439.06*	*422.37*	*<0.000*
B	*1314.06*	*1*	*1314.06*	*74.61*	*<0.000*
C	*430.56*	*1*	*430.56*	*24.45*	*0.0006*
AB	*1139.06*	*1*	*1139.06*	*64.67*	*<0.000*
AC	*451.56*	*1*	*451.56*	*25.64*	*0.0005*
Residual	176.12	10	17.61		
Cor Total	10950.44	15			

Std. Dev.	4.20	*R*-Squared	0.9839
Mean	399.19	Adj. *R*-Squared	0.9759
C.V.	1.05	Pred. *R*-Squared	0.9588
PRESS	450.88	Adeq. Precision	27.967

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High
Intercept	399.19	1	1.05	396.85	401.53
A-Time	21.56	1	1.05	19.22	23.90
B-Temp	9.06	1	1.05	6.72	11.40
C-Pressure	−5.19	1	1.05	−7.53	−2.85
AB	8.44	1	1.05	6.10	10.78
AC	−5.31	1	1.05	−7.65	−2.97

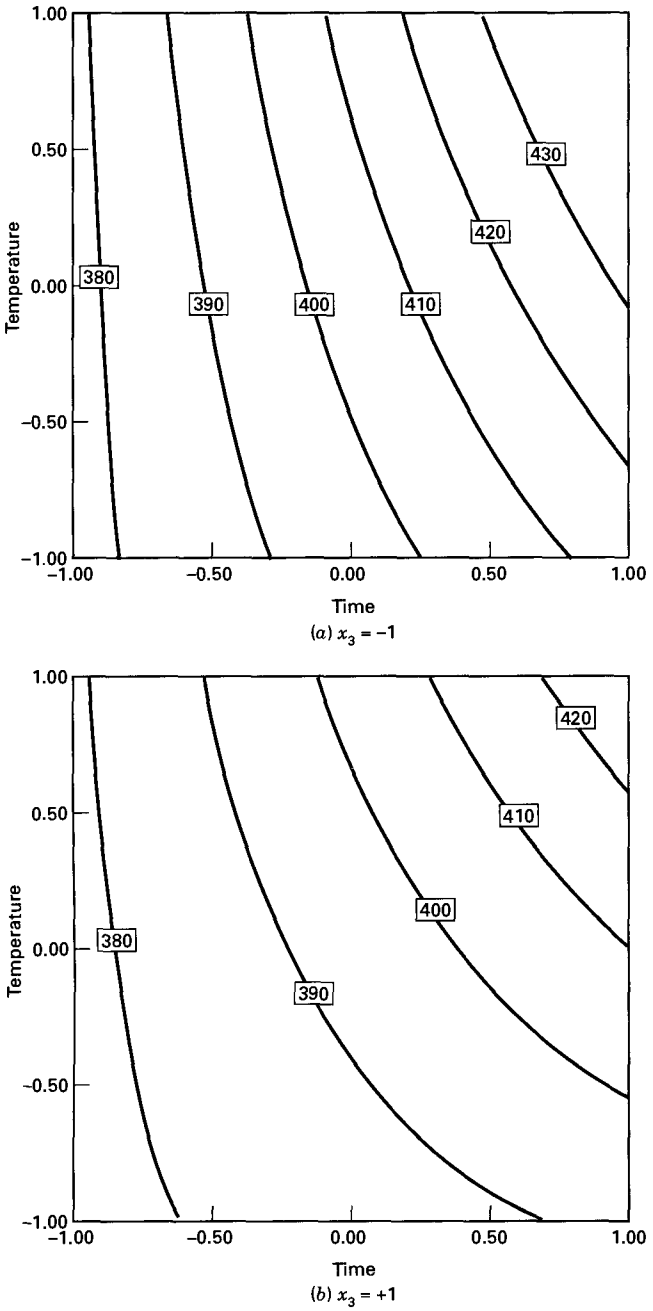


Figure 6-30 Contour plots of average oxide thickness with pressure (x_3) held constant.

important? as the incorrect analysis in Table 6-19 would certainly do. The answer is that trying to manipulate or optimize the unimportant factors would be a waste of resources, and it could result in adding unnecessary variability to *other* responses of interest.

When there are duplicate measurements on the response, there is almost always useful information about some aspect of process variability contained in these observa-

Table 6-19 Analysis of Variance (From Design-Expert) of the Individual Wafer Oxide Thickness Response

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	43801.75	15	2920.12	476.75	<0.0001
A	*29756.25*	*1*	*29756.25*	*4858.16*	*<0.0001*
B	*5256.25*	*1*	*5256.25*	*858.16*	*<0.0001*
C	*1722.25*	*1*	*1722.25*	*281.18*	*<0.0001*
D	*42.25*	*1*	*42.25*	*6.90*	*0.0115*
AB	*4556.25*	*1*	*4556.25*	*743.88*	*<0.0001*
AC	*1806.25*	*1*	*1806.25*	*294.90*	*<0.0001*
AD	*20.25*	*1*	*20.25*	*3.31*	*0.0753*
BC	*240.25*	*1*	*240.25*	*39.22*	*<0.0001*
BD	*240.25*	*1*	*240.25*	*39.22*	*<0.0001*
CD	*20.25*	*1*	*20.25*	*3.31*	*0.0753*
ABD	*132.25*	*1*	*132.25*	*21.59*	*<0.0001*
ABC	*2.25*	*1*	*2.25*	*0.37*	*0.5473*
ACD	*0.25*	*1*	*0.25*	*0.041*	*0.8407*
BCD	*6.25*	*1*	*6.25*	*1.02*	*0.3175*
ABCD	*0.25*	*1*	*0.25*	*0.041*	*0.8407*
Residual	294.00	48	6.12		
Lack of Fit	*0.000*	*0*			
Pure Error	*294.00*	*48*	*6.13*		
Cor. Total	44095.75	63			

tions. For example, if the duplicate measurements are multiple tests by a gauge on the same experimental unit, then the duplicate measurements give some insight about *gauge capability*. If the duplicate measurements are made at different locations on an experimental unit, they may give some information about the *uniformity* of the response variable across that unit. In our example, because we have one observation on each of four experimental units that have undergone processing together, we have some information about the *within-run* variability in the process. This information is contained in the variance of the oxide thickness measurements from the four wafers in each run. It would be of interest to determine if any of the process variables influence the within-run variability.

Figure 6-31 (page 270) is a normal probability plot of the effect estimates obtained using $\ln(s^2)$ as the response. Recall from Chapter 3 that we indicated that the log transformation is generally appropriate for modeling variability. There are not any strong individual effects, but factor A and the BD interaction are the largest. If we also include the main effects of B and D to obtain a hierarchical model, then the model for $\ln(s^2)$ is

$$\widehat{\ln(s^2)} = 1.08 + 0.41x_1 - 0.40x_2 + 0.20x_4 - 0.56x_2x_4$$

The model accounts for just slightly less than half of the variability in the $\ln(s^2)$ response, which is certainly not spectacular as empirical models go, but it is often difficult to obtain exceptionally good models of variances.

Figure 6-32 (page 270) is a contour plot of the predicted variance (not the log of the predicted variance) with pressure x_3 at the low level (recall that this minimizes cycle time) and gas flow x_4 at the high level. This choice of gas flow gives the lowest values of predicted variance in the region of the contour plot.

The experimenters here were interested in selecting values of the design variables that gave a mean oxide thickness within the process specifications and as close to 400 Å as possible, while simultaneously making the within-run variability small, say $s^2 \leq 2$.

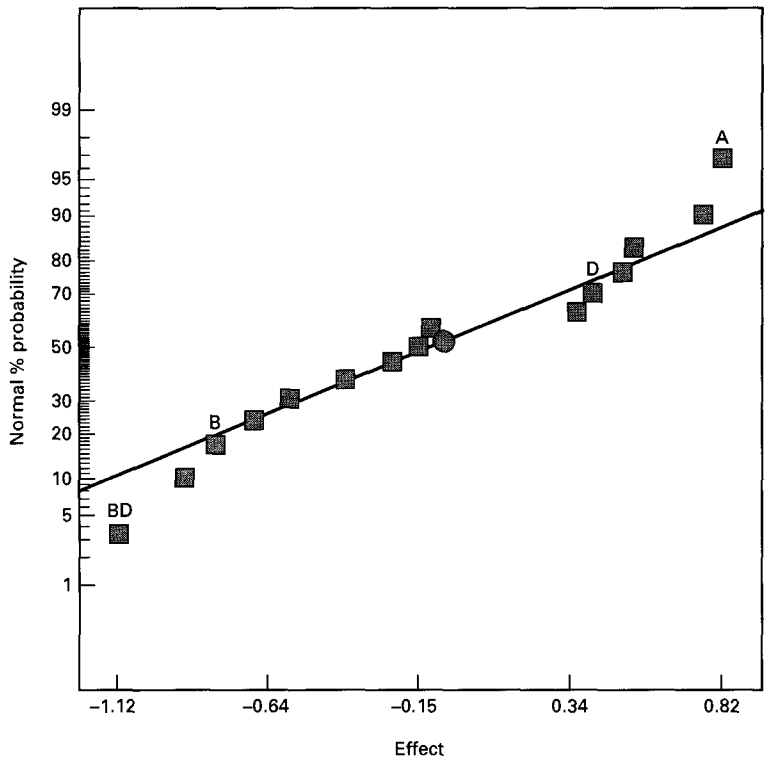


Figure 6-31 Normal probability plot of the effects using ln (s^2) as the response, Example 6-5.

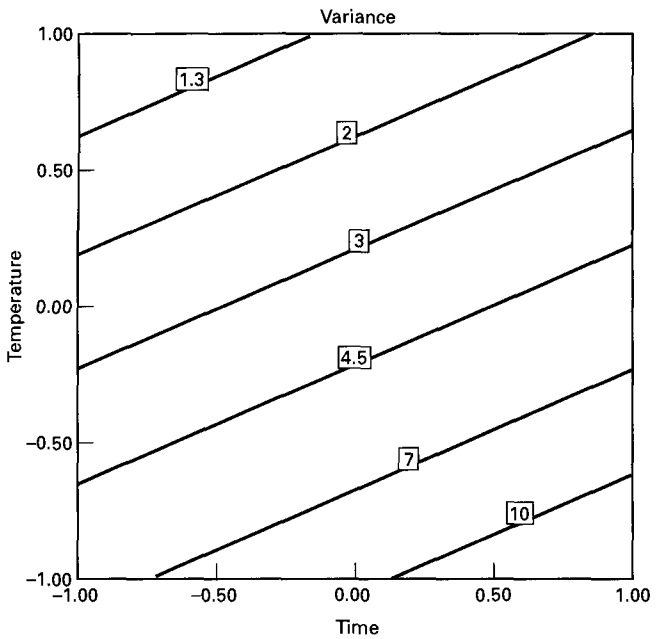


Figure 6-32 Contour plot of s^2 (within-run variability) with pressure at the low level and gas flow at the high level.

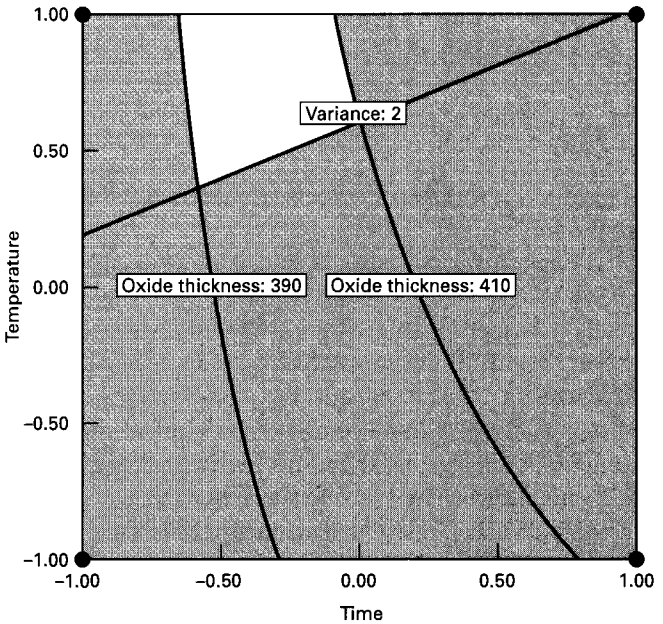


Figure 6-33 Overlay of the average oxide thickness and s^2 responses with pressure at the low level and gas flow at the high level.

One possible way to find a suitable set of conditions is to overlay the contour plots in Figures 6-30 and 6-32. The overlay plot is shown in Figure 6-33, with the specifications on mean oxide thickness and the constraint $s^2 \leq 2$ shown as contours. In this plot, pressure is held constant at the low level and gas flow is held constant at the high level. The open region near the upper left center of the graph identifies a feasible region for the variables time and temperature.

This is a simple example of using contour plots to study two responses simultaneously. We will discuss this problem in more detail in Chapter 11.

6-6 THE ADDITION OF CENTER POINTS TO THE 2^k DESIGN

A potential concern in the use of two-level factorial designs is the assumption of **linearity** in the factor effects. Of course, perfect linearity is unnecessary, and the 2^k system will work quite well even when the linearity assumption holds only very approximately. In fact, we have noted that if **interaction terms** are added to a main effects or first-order model, resulting in

$$y = \beta_0 + \sum_{j=1}^{k} \beta_j x_j + \sum\sum_{i<j} \beta_{ij} x_i x_j + \epsilon \tag{6-26}$$

then we have a model capable of representing some curvature in the response function. This curvature, of course, results from the twisting of the plane induced by the interaction terms $\beta_{ij} x_i x_j$.

There are going to be situations where the curvature in the response function is not adequately modeled by Equation 6-26. In such cases, a logical model to consider is

$$y = \beta_0 + \sum_{j=1}^{k} \beta_j x_j + \sum\sum_{i<j} \beta_{ij} x_i x_j + \sum_{j=1}^{k} \beta_{jj} x_j^2 + \epsilon \tag{6-27}$$

where the β_{jj} represent pure second-order or **quadratic effects**. Equation 6-27 is called a **second-order response surface model.**

In running a two-level factorial experiment, we usually anticipate fitting the first-order model in Equation 6-26, but we should be alert to the possibility that the second-order model in Equation 6-27 is really more appropriate. There is a method of replicating certain points in a 2^k factorial that will provide protection against curvature from second-order effects as well as allow an independent estimate of error to be obtained. The method consists of adding **center points** to the 2^k design. These consist of n replicates run at the points $x_i = 0$ $(i = 1, 2, \ldots, k)$. One important reason for adding the replicate runs at the design center is that center points do not affect the usual effect estimates in a 2^k design. When we add center points, we assume that the k factors are **quantitative.**

To illustrate the approach, consider a 2^2 design with one observation at each of the factorial points $(-, -)$, $(+, -)$, $(-, +)$ and $(+, +)$ and n_C observations at the center point $(0, 0)$. Figure 6-34 illustrates the situation. Let $\bar{y}_F$ be the average of the four runs at the four factorial points and let $\bar{y}_C$ be the average of the n_C runs at the center point. If the difference $\bar{y}_F - \bar{y}_C$ is small, then the center points lie on or near the plane passing through the factorial points, and there is no quadratic curvature. On the other hand, if $\bar{y}_F - \bar{y}_C$ is large, then quadratic curvature is present. A single-degree-of-freedom **sum of squares for pure quadratic curvature** is given by

$$SS_{\text{Pure quadratic}} = \frac{n_F n_C (\bar{y}_F - \bar{y}_C)^2}{n_F + n_C} \tag{6-28}$$

where, in general, n_F is the number of factorial design points. This quantity may be compared to the error mean square to test for pure quadratic curvature. More specifically,

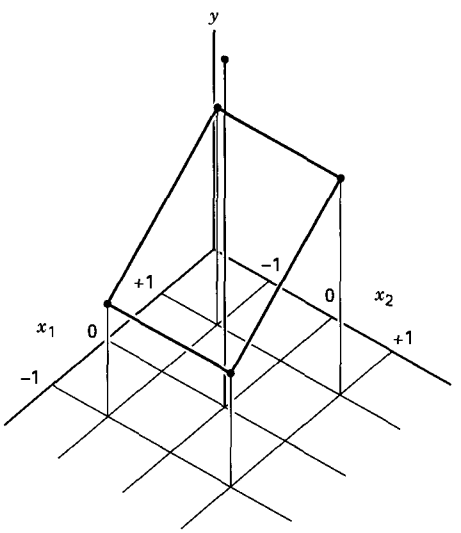


Figure 6-34 A 2^2 design with center points.

when points are added to the center of the 2^k design, then the test for curvature (using Equation 6-28) actually tests the hypotheses

$$H_0: \sum_{j=1}^{k} \beta_{jj} = 0$$

$$H_1: \sum_{j=1}^{k} \beta_{jj} \neq 0$$

Furthermore, if the factorial points in the design are unreplicated, one may use the n_C center points to construct an estimate of error with $n_C - 1$ degrees of freedom.

EXAMPLE 6-6

A chemical engineer is studying the yield of a process. There are two variables of interest, reaction time and reaction temperature. Because she is uncertain about the assumption of linearity over the region of exploration, the engineer decides to conduct a 2^2 design (with a single replicate of each factorial run) augmented with five center points. The design and the yield data are shown in Figure 6-35.

Table 6-20 summarizes the analysis of variance for this experiment. The mean square error is calculated from the center points as follows:

$$MS_E = \frac{SS_E}{n_C - 1} = \frac{\sum_{\text{Center points}} (y_i - \bar{y})^2}{n_C - 1} \tag{6-29}$$

Thus, in Table 6-20 (page 274),

$$MS_E = \frac{\sum_{i=1}^{5} (y_i - 40.46)^2}{4} = \frac{0.1720}{4} = 0.0430$$

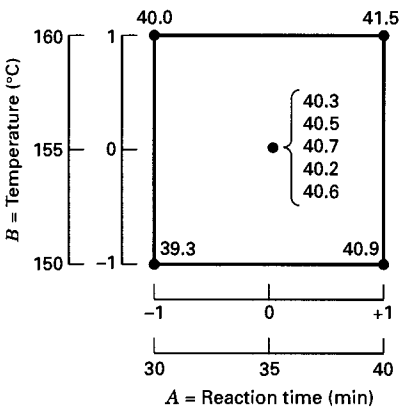


Figure 6-35 The 2^2 design with five center points for Example 6-6.

Table 6-20 Analysis of Variance for Example 6-6

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
A (Time)	2.4025	1	2.4025	55.87	0.0017
B (Temperature)	0.4225	1	0.4225	9.83	0.0350
AB	0.0025	1	0.0025	0.06	0.8185
Pure quadratic	0.0027	1	0.0027	0.06	0.8185
Error	0.1720	4	0.0430		
Total	3.0022	8			

The average of the points in the factorial portion of the design is $\bar{y}_F = 40.425$, and the average of the points at the center is $\bar{y}_C = 40.46$. The difference $\bar{y}_F - \bar{y}_C = 40.425 - 40.46 = -0.035$ appears to be small. The pure quadratic curvature sum of squares in the analysis of variance table is computed from Equation 6-28 as follows:

$$\begin{aligned} SS_{\text{Pure quadratic}} &= \frac{n_F n_C (\bar{y}_F - \bar{y}_C)^2}{n_F + n_C} \\ &= \frac{(4)(5)(-0.035)^2}{4 + 5} \\ &= 0.0027 \end{aligned}$$

The analysis of variance indicates that both factors exhibit significant main effects, that there is no interaction, and that there is no evidence of second-order curvature in the response over the region of exploration. That is, the null hypothesis $H_0: \beta_{11} + \beta_{22} = 0$ cannot be rejected.

In Example 6-6, we concluded that there was no indication of quadratic effects; that is, a first-order model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \epsilon$$

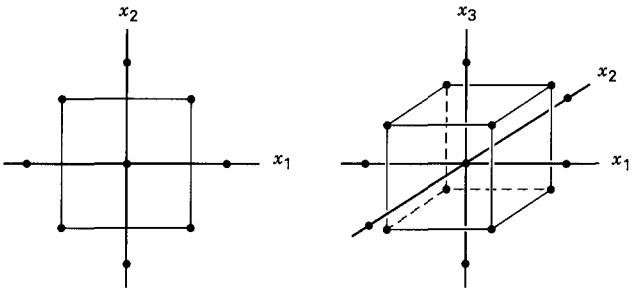
is appropriate (although we probably don't need the interaction term). There will be situations where the quadratic terms will be required. That is, we will now have to assume a second-order model such as

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \epsilon$$

Unfortunately, we cannot estimate the unknown parameters (the β's) in this model because there are six parameters to estimate and the 2^2 design plus center points in Figure 6-35 only has five independent runs.

A simple and highly effective solution to this problem is to augment the 2^2 design with four **axial runs**, as shown in Figure 6-36*a*. The resulting design, called a **central composite design**, can now be used to fit the second-order model. Figure 6-36*b* shows a central composite design for $k = 3$ factors. This design has $14 + n_C$ runs (usually $3 \leq n_C \leq 5$), and is a very efficient design for fitting the 10-parameter second-order model in $k = 3$ factors.

Central composite designs are used extensively in building second-order response surface models. These designs will be discussed in more detail in Chapter 11.



(*a*) Two factors (*b*) Three factors

Figure 6-36 Central composite designs.

We conclude this section with a few additional useful suggestions and observations concerning the use of center points.

1. When a factorial experiment is conducted in an ongoing process, consider using the current operating conditions (or recipe) as the center point in the design. This often assures the operating personnel that at least some of the runs in the experiment are going to be performed under familiar conditions, and so the results obtained (at least for these runs) are unlikely to be any worse than are typically obtained.
2. When the center point in a factorial experiment correspond to the usual operating recipe, the experimenter can use the observed responses at the center point to provide a rough check of whether anything "unusual" occurred during the experiment. That is, the center point responses should be very similar to responses observed historically in routine process operation. Often operating personnel will maintain a control chart for monitoring process performance. Sometimes the center point responses can be plotted directly on the control chart as a check of the manner in which the process was operating during the experiment.
3. Consider running the replicates at the center point in nonrandom order. Specifically, run one or two center points at or near the beginning of the experiment, one or two near the middle, and one or two near the end. By spreading the center points out in time, the experimenter has a rough check on the stability of the process during the experiment. For example, if a trend has occurred in the response while the experiment was performed, plotting the center point responses versus time order may reveal this.
4. Sometimes experiments must be conducted in situations where there is little or no prior information about process variability. In these cases, running two or three center points as the first few runs in the experiment can be very helpful. These runs can provide a preliminary estimate of variability. If the magnitude of the variability seems reasonable, continue; on the other hand, if larger than anticipated (or reasonable!) variability is observed, stop. Often it will be very profitable to study the question of why the variability is so large before proceeding with the rest of the experiment.
5. Usually, center points are employed when all design factors are **quantitative**. However, sometimes there will be one or more qualitative or categorical variables and several quantitative ones. Center points can still be employed in these cases.

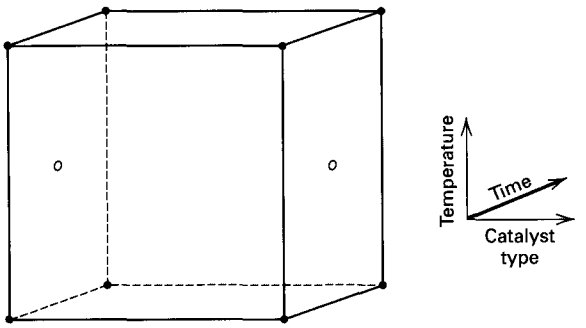


Figure 6-37 A 2^3 factorial design with one qualitative factor and center points.

To illustrate, consider an experiment with two quantitative factors, time and temperature, each at two levels, and a single qualitative factor, catalyst type, also with two levels (organic and nonorganic). Figure 6-37 shows the 2^3 design for these factors. Notice that the center points are placed in the opposed faces of the cube which involve the quantitative factors. In other words, the center points can be run at the high and low level treatment combinations of the qualitative factors, just so long as those subspaces involves only quantitative factors.

6-7 PROBLEMS

6-1. An engineer is interested in the effects of cutting speed (A), tool geometry (B), and cutting angle (C) on the life (in hours) of a machine tool. Two levels of each factor are chosen, and three replicates of a 2^3 factorial design are run. The results follow:

			Treatment	Replicate		
A	B	C	Combination	I	II	III
−	−	−	(1)	22	31	25
+	−	−	a	32	43	29
−	+	−	b	35	34	50
+	+	−	ab	55	47	46
−	−	+	c	44	45	38
+	−	+	ac	40	37	36
−	+	+	bc	60	50	54
+	+	+	abc	39	41	47

(a) Estimate the factor effects. Which effects appear to be large?
(b) Use the analysis of variance to confirm your conclusions for part (a).
(c) Write down a regression model for predicting tool life (in hours) based on the results of this experiment.
(d) Analyze the residuals. Are there any obvious problems?
(e) Based on an analysis of main effect and interaction plots, what levels of A, B, and C would you recommend using?

6-2. Reconsider part (c) of Problem 6-1. Use the regression model to generate response surface and contour plots of the tool life response. Interpret these plots. Do they provide insight regarding the desirable operating conditions for this process?

6-3. Find the standard error of the factor effects and approximate 95 percent confidence limits for the factor effects in Problem 6-1. Do the results of this analysis agree with the conclusions from the analysis of variance?

6-4. Plot the factor effects from Problem 6-1 on a graph relative to an appropriately scaled t distribution. Does this graphical display adequately identify the important factors? Compare the conclusions from this plot with the results from the analysis of variance.

6-5. A router is used to cut locating notches on a printed circuit board. The vibration level at the surface of the board as it is cut is considered to be a major source of dimensional variation in the notches. Two factors are thought to influence vibration: bit size (A) and cutting speed (B). Two bit sizes ($\frac{1}{16}$ and $\frac{1}{8}$ inch) and two speeds (40 and 90 rpm) are selected, and four boards are cut at each set of conditions shown below. The response variable is vibration measured as the resultant vector of three accelerometers (x, y, and z) on each test circuit board.

		Treatment	Replicate			
A	B	Combination	I	II	III	IV
−	−	(1)	18.2	18.9	12.9	14.4
+	−	a	27.2	24.0	22.4	22.5
−	+	b	15.9	14.5	15.1	14.2
+	+	ab	41.0	43.9	36.3	39.9

(a) Analyze the data from this experiment.
(b) Construct a normal probability plot of the residuals, and plot the residuals versus the predicted vibration level. Interpret these plots.
(c) Draw the AB interaction plot. Interpret this plot. What levels of bit size and speed would you recommend for routine operation?

6-6. Reconsider the experiment described in Problem 6-1. Suppose that the experimenter only performed the eight trials from replicate I. In addition, he ran four center points and obtained the following response values: 36, 40, 43, 45.
(a) Estimate the factor effects. Which effects are large?
(b) Perform an analysis of variance, including a check for pure quadratic curvature. What are your conclusions?
(c) Write down an appropriate model for predicting tool life, based on the results of this experiment. Does this model differ in any substantial way from the model in Problem 6-1, part (c)?
(d) Analyze the residuals.
(e) What conclusions would you draw about the appropriate operating conditions for this process?

6-7. An experiment was performed to improve the yield of a chemical process. Four factors were selected, and two replicates of a completely randomized experiment were run. The results are shown in the following table:

Treatment	Replicate		Treatment	Replicate	
Combination	I	II	Combination	I	II
(1)	90	93	d	98	95
a	74	78	ad	72	76
b	81	85	bd	87	83
ab	83	80	abd	85	86
c	77	78	cd	99	90
ac	81	80	acd	79	75
bc	88	82	bcd	87	84
abc	73	70	$abcd$	80	80

(a) Estimate the factor effects.
(b) Prepare an analysis of variance table, and determine which factors are important in explaining yield.
(c) Write down a regression model for predicting yield, assuming that all four factors were varied over the range from -1 to $+1$ (in coded units).
(d) Plot the residuals versus the predicted yield and on a normal probability scale. Does the residual analysis appear satisfactory?
(e) Two three-factor interactions, ABC and ABD, apparently have large effects. Draw a cube plot in the factors A, B, and C with the average yields shown at each corner. Repeat using the factors A, B, and D. Do these two plots aid in data interpretation? Where would you recommend that the process be run with respect to the four variables?

6-8. A bacteriologist is interested in the effects of two different culture media and two different times on the growth of a particular virus. She performs six replicates of a 2^2 design, making the runs in random order. Analyze the bacterial growth data that follow and draw appropriate conclusions. Analyze the residuals and comment on the model's adequacy.

	Culture Medium			
Time, h	1		2	
12	21	22	25	26
	23	28	24	25
	20	26	29	27
18	37	39	31	34
	38	38	29	33
	35	36	30	35

6-9. An industrial engineer employed by a beverage bottler is interested in the effects of two different types of 32-ounce bottles on the time to deliver 12-bottle cases of the product. The two bottle types are glass and plastic. Two workers are used to perform a task consisting of moving 40 cases of the product 50 feet on a standard type of hand truck and stacking the cases in a display. Four replicates of a 2^2 factorial design are performed, and the times observed are listed in the following table. Analyze the data and draw appropriate conclusions. Analyze the residuals and comment on the model's adequacy.

	Worker			
Bottle Type	1		2	
Glass	5.12	4.89	6.65	6.24
	4.98	5.00	5.49	5.55
Plastic	4.95	4.43	5.28	4.91
	4.27	4.25	4.75	4.71

6-10. In Problem 6-9, the engineer was also interested in potential fatigue differences resulting from the two types of bottles. As a measure of the amount of effort required, he measured the elevation of the heart rate (pulse) induced by the task. The results follow. Analyze the data and draw conclusions. Analyze the residuals and comment on the model's adequacy.

Bottle Type	Worker 1		Worker 2	
Glass	39	45	20	13
	58	35	16	11
Plastic	44	35	13	10
	42	21	16	15

6-11. Calculate approximate 95 percent confidence limits for the factor effects in Problem 6-10. Do the results of this analysis agree with the analysis of variance performed in Problem 6-10?

6-12. An article in the *AT&T Technical Journal* (March/April 1986, Vol. 65, pp. 39–50) describes the application of two-level factorial designs to integrated circuit manufacturing. A basic processing step is to grow an epitaxial layer on polished silicon wafers. The wafers mounted on a susceptor are positioned inside a bell jar, and chemical vapors are introduced. The susceptor is rotated and heat is applied until the epitaxial layer is thick enough. An experiment was run using two factors: arsenic flow rate (A) and deposition time (B). Four replicates were run, and the epitaxial layer thickness was measured (in μm). The data are shown below:

A	B	Replicate I	II	III	IV		Factor Levels Low (−)	High (+)
−	−	14.037	16.165	13.972	13.907	A	55%	59%
+	−	13.880	13.860	14.032	13.914			
−	+	14.821	14.757	14.843	14.878	B	Short	Long
+	+	14.888	14.921	14.415	14.932		(10 min)	(15 min)

(a) Estimate the factor effects.
(b) Conduct an analysis of variance. Which factors are important?
(c) Write down a regression equation that could be used to predict epitaxial layer thickness over the region of arsenic flow rate and deposition time used in this experiment.
(d) Analyze the residuals. Are there any residuals that should cause concern?
(e) Discuss how you might deal with the potential outlier found in part (d).

6-13. ***Continuation of Problem 6-12.*** Use the regression model in part (c) of Problem 6-12 to generate a response surface contour plot for epitaxial layer thickness. Suppose it is critically important to obtain layer thickness of 14.5 μm. What settings of arsenic flow rate and decomposition time would you recommend?

6-14. ***Continuation of Problem 6-13.*** How would your answer to Problem 6-13 change if arsenic flow rate was more difficult to control in the process than the deposition time?

6-15. A nickel-titanium alloy is used to make components for jet turbine aircraft engines. Cracking is a potentially serious problem in the final part, because it can lead to nonrecoverable failure. A test is run at the parts producer to determine the effect of four factors on cracks. The four factors are pouring temperature (A), titanium content (B), heat treatment method (C), and amount of grain refiner used (D). Two replicates of a 2^4 design are run, and the length of crack (in mm $\times 10^{-2}$) induced in a sample coupon subjected to a standard test is measured. The data are shown in the following table:

A	B	C	D	Treatment Combination	Replicate I	Replicate II
−	−	−	−	(1)	7.037	6.376
+	−	−	−	*a*	14.707	15.219
−	+	−	−	*b*	11.635	12.089
+	+	−	−	*ab*	17.273	17.815
−	−	+	−	*c*	10.403	10.151
+	−	+	−	*ac*	4.368	4.098
−	+	+	−	*bc*	9.360	9.253
+	+	+	−	*abc*	13.440	12.923
−	−	−	+	*d*	8.561	8.951
+	−	−	+	*ad*	16.867	17.052
−	+	−	+	*bd*	13.876	13.658
+	+	−	+	*abd*	19.824	19.639
−	−	+	+	*cd*	11.846	12.337
+	−	+	+	*acd*	6.125	5.904
−	+	+	+	*bcd*	11.190	10.935
+	+	+	+	*abcd*	15.653	15.053

(a) Estimate the factor effects. Which factor effects appear to be large?
(b) Conduct an analysis of variance. Do any of the factors affect cracking? Use $\alpha = 0.05$.
(c) Write down a regression model that can be used to predict crack length as a function of the significant main effects and interactions you have identified in part (b).
(d) Analyze the residuals from this experiment.
(e) Is there an indication that any of the factors affect the variability in cracking?
(f) What recommendations would you make regarding process operations? Use interaction and/or main effect plots to assist in drawing conclusions.

6-16. ***Continuation of Problem 6-15.*** One of the variables in the experiment described in Problem 6-15, heat treatment method (C), is a categorical variable. Assume that the remaining factors are continuous.
(a) Write two regression models for predicting crack length, one for each level of the heat treatment method variable. What differences, if any, do you notice in these two equations?
(b) Generate appropriate response surface contour plots for the two regression models in part (a).
(c) What set of conditions would you recommend for the factors A, B, and D if you use heat treatment method $C = +$?
(d) Repeat part (c) assuming that you wish to use heat treatment method $C = -$.

6-17. An experimenter has run a single replicate of a 2^4 design. The following effect estimates have been calculated:

$A = 76.95$	$AB = -51.32$	$ABC = -2.82$
$B = -67.52$	$AC = 11.69$	$ABD = -6.50$
$C = -7.84$	$AD = 9.78$	$ACD = 10.20$
$D = -18.73$	$BC = 20.78$	$BCD = -7.98$
	$BD = 14.74$	$ABCD = -6.25$
	$CD = 1.27$	

(a) Construct a normal probability plot of these effects.
(b) Identify a tentative model, based on the plot of the effects in part (a).

6-18. An article in *Solid State Technology* ("Orthogonal Design for Process Optimization and Its Application in Plasma Etching," May 1987, pp. 127–132) describes the application of factorial designs in developing a nitride etch process on a single-wafer plasma etcher. The process uses C_2F_6 as the reactant gas. Four factors are of interest: anode–cathode gap (A), pressure in the reactor chamber (B), C_2F_6 gas flow (C), and power applied to the cathode (D). The response variable of interest is the etch rate for silicon nitride. A single replicate of a 2^4 design is run, and the data are shown below:

Run Number	Actual Run Order	A	B	C	D	Etch Rate (Å/min)
1	13	−	−	−	−	550
2	8	+	−	−	−	669
3	12	−	+	−	−	604
4	9	+	+	−	−	650
5	4	−	−	+	−	633
6	15	+	−	+	−	642
7	16	−	+	+	−	601
8	3	+	+	+	−	635
9	1	−	−	−	+	1037
10	14	+	−	−	+	749
11	5	−	+	−	+	1052
12	10	+	+	−	+	868
13	11	−	−	+	+	1075
14	2	+	−	+	+	860
15	7	−	+	+	+	1063
16	6	+	+	+	+	729

Factor Levels	Low (−)	High (+)
A (cm)	0.80	1.20
B (mTorr)	450	550
C (SCCM)	125	200
D (W)	275	325

(a) Estimate the factor effects. Consider a normal probability plot of the factor effects. Which effects appear large?
(b) Conduct an analysis of variance to confirm your findings for part (a).
(c) What is the regression model relating etch rate to the significant process variables?
(d) Analyze the residuals from this experiment. Comment on the model's adequacy.
(e) If not all the factors are important, project the 2^4 design into a 2^k design with $k < 4$ and conduct the analysis of variance.
(f) Draw graphs to interpret any significant interactions.
(g) Plot the residuals versus the actual run order. What problems might be revealed by this plot?

6-19. ***Continuation of Problem 6-18.*** Consider the regression model obtained in part (c) of Problem 6-18.
(a) Construct contour plots of the etch rate using this model.
(b) Suppose that it was necessary to operate this process at an etch rate of 800 Å/min. What settings of the process variables would you recommend?

6-20. Consider the single replicate of the 2^4 design in Example 6-2. Suppose we had arbitrarily decided to analyze the data assuming that all three- and four-factor interactions were negligible. Conduct this analysis and compare your results with those obtained in the example. Do you think that it is a good idea to arbitrarily assume interactions to be negligible even if they are relatively high-order ones?

6-21. An experiment was run in a semiconductor fabrication plant in an effort to increase yield. Five factors, each at two levels, were studied. The factors (and levels) were A = aperture setting (small, large), B = exposure time (20% below nominal, 20% above nominal),

C = development time (30 s, 45 s), D = mask dimension (small, large), and E = etch time (14.5 min, 15.5 min). The unreplicated 2^5 design shown below was run.

$(1) = 7$	$d = 8$	$e = 8$	$de = 6$
$a = 9$	$ad = 10$	$ae = 12$	$ade = 10$
$b = 34$	$bd = 32$	$be = 35$	$bde = 30$
$ab = 55$	$abd = 50$	$abe = 52$	$abde = 53$
$c = 16$	$cd = 18$	$ce = 15$	$cde = 15$
$ac = 20$	$acd = 21$	$ace = 22$	$acde = 20$
$bc = 40$	$bcd = 44$	$bce = 45$	$bcde = 41$
$abc = 60$	$abcd = 61$	$abce = 65$	$abcde = 63$

(a) Construct a normal probability plot of the effect estimates. Which effects appear to be large?
(b) Conduct an analysis of variance to confirm your findings for part (a).
(c) Write down the regression model relating yield to the significant process variables.
(d) Plot the residuals on normal probability paper. Is the plot satisfactory?
(e) Plot the residuals versus the predicted yields and versus each of the five factors. Comment on the plots.
(f) Interpret any significant interactions.
(g) What are your recommendations regarding process operating conditions?
(h) Project the 2^5 design in this problem into a 2^k design in the important factors. Sketch the design and show the average and range of yields at each run. Does this sketch aid in interpreting the results of this experiment?

6-22. ***Continuation of Problem 6-21.*** Suppose that the experimenter had run four center points in addition to the 32 trials in the original experiment. The yields obtained at the center point runs were 68, 74, 76, and 70.
(a) Reanalyze the experiment, including a test for pure quadratic curvature.
(b) Discuss what your next step would be.

6-23. In a process development study on yield, four factors were studied, each at two levels: time (A), concentration (B), pressure (C), and temperature (D). A single replicate of a 2^4 design was run, and the resulting data are shown in the following table:

Run Number	Actual Run Order	A	B	C	D	Yield (lbs)	Factor Levels	
							Low (−)	High (+)
1	5	−	−	−	−	12	A (h) 2.5	3
2	9	+	−	−	−	18	B (%) 14	18
3	8	−	+	−	−	13	C (psi) 60	80
4	13	+	+	−	−	16	D (°C) 225	250
5	3	−	−	+	−	17		
6	7	+	−	+	−	15		
7	14	−	+	+	−	20		
8	1	+	+	+	−	15		
9	6	−	−	−	+	10		
10	11	+	−	−	+	25		
11	2	−	+	−	+	13		
12	15	+	+	−	+	24		
13	4	−	−	+	+	19		
14	16	+	−	+	+	21		
15	10	−	+	+	+	17		
16	12	+	+	+	+	23		

(a) Construct a normal probability plot of the effect estimates. Which factors appear to have large effects?
(b) Conduct an analysis of variance using the normal probability plot in part (a) for guidance in forming an error term. What are your conclusions?
(c) Write down a regression model relating yield to the important process variables.
(d) Analyze the residuals from this experiment. Does your analysis indicate any potential problems?
(e) Can this design be collapsed into a 2^3 design with two replicates? If so, sketch the design with the average and range of yield shown at each point in the cube. Interpret the results.

6-24. ***Continuation of Problem 6-23.*** Use the regression model in part (c) of Problem 6-23 to generate a response surface contour plot of yield. Discuss the practical value of this response surface plot.

6-25. ***The scrumptious brownie experiment.*** The author is an engineer by training and a firm believer in learning by doing. I have taught experimental design for many years to a wide variety of audiences and have always assigned the planning, conduct, and analysis of an actual experiment to the class participants. The participants seem to enjoy this practical experience and always learn a great deal from it. This problem uses the results of an experiment performed by Gretchen Krueger at Arizona State University.

There are many different ways to bake brownies. The purpose of this experiment was to determine how the pan material, the brand of brownie mix, and the stirring method affect the scrumptiousness of brownies. The factor levels were

Factor	Low (−)	High (+)
A = pan material	Glass	Aluminum
B = stirring method	Spoon	Mixer
C = brand of mix	Expensive	Cheap

The response variable was scrumptiousness, a subjective measure derived from a questionnaire given to the subjects who sampled each batch of brownies. (The questionnaire dealt with such issues as taste, appearance, consistency, aroma, and so forth). An eight-person test panel sampled each batch and filled out the questionnaire. The design matrix and the response data are shown below:

Brownie Batch	A	B	C	Test Panel Results							
				1	2	3	4	5	6	7	8
1	−	−	−	11	9	10	10	11	10	8	9
2	+	−	−	15	10	16	14	12	9	6	15
3	−	+	−	9	12	11	11	11	11	11	12
4	+	+	−	16	17	15	12	13	13	11	11
5	−	−	+	10	11	15	8	6	8	9	14
6	+	−	+	12	13	14	13	9	13	14	9
7	−	+	+	10	12	13	10	7	7	17	13
8	+	+	+	15	12	15	13	12	12	9	14

(a) Analyze the data from this experiment as if there were eight replicates of a 2^3 design. Comment on the results.

(b) Is the analysis in part (a) the correct approach? There are only eight batches; do we really have eight replicates of a 2^3 factorial design?

(c) Analyze the average and standard deviation of the scrumptiousness ratings. Comment on the results. Is this analysis more appropriate than the one in part (a)? Why or why not?

6-26. An experiment was conducted on a chemical process that produces a polymer. The four factors studied were temperature (A), catalyst concentration (B), time (C), and pressure (D). Two responses, molecular weight and viscosity, were observed. The design matrix and response data are shown below:

Run Number	Actual Run Order	A	B	C	D	Molecular Weight	Viscosity	Factor Levels Low (−)	Factor Levels High (+)
1	18	−	−	−	−	2400	1400	A (°C) 100	120
2	9	+	−	−	−	2410	1500	B (%) 4	8
3	13	−	+	−	−	2315	1520	C (min) 20	30
4	8	+	+	−	−	2510	1630	D (psi) 60	75
5	3	−	−	+	−	2615	1380		
6	11	+	−	+	−	2625	1525		
7	14	−	+	+	−	2400	1500		
8	17	+	+	+	−	2750	1620		
9	6	−	−	−	+	2400	1400		
10	7	+	−	−	+	2390	1525		
11	2	−	+	−	+	2300	1500		
12	10	+	+	−	+	2520	1500		
13	4	−	−	+	+	2625	1420		
14	19	+	−	+	+	2630	1490		
15	15	−	+	+	+	2500	1500		
16	20	+	+	+	+	2710	1600		
17	1	0	0	0	0	2515	1500		
18	5	0	0	0	0	2500	1460		
19	16	0	0	0	0	2400	1525		
20	12	0	0	0	0	2475	1500		

(a) Consider only the molecular weight response. Plot the effect estimates on a normal probability scale. What effects appear important?

(b) Use an analysis of variance to confirm the results from part (a). Is there indication of curvature?

(c) Write down a regression model to predict molecular weight as a function of the important variables.

(d) Analyze the residuals and comment on model adequacy.

(e) Repeat parts (a)–(d) using the viscosity response.

6-27. ***Continuation of Problem 6-26.*** Use the regression models for molecular weight and viscosity to answer the following questions.

(a) Construct a response surface contour plot for molecular weight. In what direction would you adjust the process variables to increase molecular weight?

(b) Construct a response surface contour plot for viscosity. In what direction would you adjust the process variables to decrease viscosity?

(c) What operating conditions would you recommend if it was necessary to produce a product with molecular weight between 2400 and 2500, and the lowest possible viscosity?

6-28. Consider the single replicate of the 2^4 design in Example 6-2. Suppose that we ran five points at the center (0, 0, 0, 0) and observed the following responses: 73, 75, 71, 69, and 76. Test for curvature in this experiment. Interpret the results.

6-29. ***A missing value in a 2^k factorial.*** It is not unusual to find that one of the observations in a 2^k design is missing due to faulty measuring equipment, a spoiled test, or some other reason. If the design is replicated n times ($n > 1$) some of the techniques discussed in Chapter 5 can be employed. However, for an unreplicated factorial ($n = 1$) some other method must be used. One logical approach is to estimate the missing value with a number that makes the highest-order interaction contrast zero. Apply this technique to the experiment in Example 6-2 assuming that run *ab* is missing. Compare the results with the results of Example 6-2.

6-30. An engineer has performed an experiment to study the effect of four factors on the surface roughness of a machined part. The factors (and their levels) are A = tool angle (12, 15°), B = cutting fluid viscosity (300, 400), C = feed rate (10, 15 in/min), and D = cutting fluid cooler used (no, yes). The data from this experiment (with the factors coded to the usual -1, $+1$ levels) are shown below.

Run	A	B	C	D	Surface Roughness
1	−	−	−	−	0.00340
2	+	−	−	−	0.00362
3	−	+	−	−	0.00301
4	+	+	−	−	0.00182
5	−	−	+	−	0.00280
6	+	−	+	−	0.00290
7	−	+	+	−	0.00252
8	+	+	+	−	0.00160
9	−	−	−	+	0.00336
10	+	−	−	+	0.00344
11	−	+	−	+	0.00308
12	+	+	−	+	0.00184
13	−	−	+	+	0.00269
14	+	−	+	+	0.00284
15	−	+	+	+	0.00253
16	+	+	+	+	0.00163

(a) Estimate the factor effects. Plot the effect estimates on a normal probability plot and select a tentative model.

(b) Fit the model identified in part (a) and analyze the residuals. Is there any indication of model inadequacy?

(c) Repeat the analysis from parts (a) and (b) using $1/y$ as the response variable. Is there an indication that the transformation has been useful?

(d) Fit a model in terms of the coded variables that can be used to predict the surface roughness. Convert this prediction equation into a model in the natural variables.

6-31. Resistivity on a silicon wafer is influenced by several factors. The results of a 2^4 factorial experiment performed during a critical processing step is shown in the following table:

Run	A	B	C	D	Resistivity
1	−	−	−	−	1.92
2	+	−	−	−	11.28
3	−	+	−	−	1.09
4	+	+	−	−	5.75
5	−	−	+	−	2.13
6	+	−	+	−	9.53
7	−	+	+	−	1.03
8	+	+	+	−	5.35
9	−	−	−	+	1.60
10	+	−	−	+	11.73
11	−	+	−	+	1.16
12	+	+	−	+	4.68
13	−	−	+	+	2.16
14	+	−	+	+	9.11
15	−	+	+	+	1.07
16	+	+	+	+	5.30

(a) Estimate the factor effects. Plot the effect estimates on a normal probability plot and select a tentative model.

(b) Fit the model identified in part (a) and analyze the residuals. Is there any indication of model inadequacy?

(c) Repeat the analysis from parts (a) and (b) using ln (y) as the response variable. Is there an indication that the transformation has been useful?

(d) Fit a model in terms of the coded variables that can be used to predict the resistivity.

6-32. ***Continuation of Problem 6-31.*** Suppose that the experimenter had also run four center points along with the 16 runs in Problem 6-31. The resistivity measurements at the center points are 8.15, 7.63, 8.95, and 6.48. Analyze the experiment again incorporating the center points. What conclusions can you draw now?

6-33. Often the fitted regression model from a 2^k factorial design is used to make predictions at points of interest in the design space.

(a) Find the variance of the predicted response $\hat{y}$ at a point $x_1, x_2, \ldots, x_k$ in the design space. Hint: Remember that the x's are coded variables, and assume a 2^k design with an equal number of replicates n at each design point so that the variance of a regression coefficient $\hat{\beta}$ is $\sigma^2/(n2^k)$ and that the covariance between any pair of regression coefficients is zero.

(b) Use the result in part (a) to find an equation for a $100(1 - \alpha)$ percent confidence interval on the true mean response at the point $x_1, x_2, \ldots, x_k$ in design space.

6-34. ***Hierarchial models.*** Several times we have used the hierarchy principle in selecting a model; that is, we have included nonsignificant lower-order terms in a model because they were factors involved in significant higher-order terms. Hierarchy is certainly not an absolute principle that must be followed in all cases. To illustrate, consider the model resulting from Problem 6-1, which required that a nonsignificant main effect be included to achieve hierarchy. Using the data from Problem 6-1,

(a) Fit both the hierarchial and the nonhierarchial model.

(b) Calculate the PRESS statistic, the adjusted R^2, and the mean square error for both models.

(c) Find a 95 percent confidence interval on the estimate of the mean response at a cube corner ($x_1 = x_2 = x_3 = \pm 1$). Hint: Use the results of Problem 6-33.

(d) Based on the analyses you have conducted, which model do you prefer?

7 Blocking and Confounding in the 2^k Factorial Design

7-1 INTRODUCTION

There are many situations in which it is impossible to perform all of the runs in a 2^k factorial experiment under homogeneous conditions. For example, a single batch of raw material might not be large enough to make all of the required runs. In other cases, it might be desirable to deliberately vary the experimental conditions to ensure that the treatments are equally effective (that is, are robust) across many situations that are likely to be encountered in practice. For example, a chemical engineer may run a pilot plant experiment with several batches of raw material because he knows that different raw material batches of different quality grades are likely to be used in the actual full-scale process.

The design technique used in these situations is **blocking**. In this chapter, we will concentrate on some special techniques for blocking in the 2^k factorial design.

7-2 BLOCKING A REPLICATED 2^k FACTORIAL DESIGN

Suppose that the 2^k factorial design has been replicated n times. This is identical to the situation discussed in Chapter 5, where we showed how to run a general factorial design in blocks. If there are n replicates, then each set of nonhomogeneous conditions defines a block, and each replicate is run in one of the blocks. The runs in each block (or replicate)

Table 7-1 Chemical Process Experiment in Three Blocks

	Block 1	Block 2	Block 3
	(1) = 28	(1) = 25	(1) = 27
	a = 36	a = 32	a = 32
	b = 18	b = 19	b = 23
	ab = 31	ab = 30	ab = 29
Block totals:	$B_1 = 113$	$B_2 = 106$	$B_3 = 111$

Table 7-2 Analysis of Variance for the Chemical Process Experiment in Three Blocks

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Blocks	6.50	2	3.25		
A (concentration)	208.33	1	208.33	50.32	0.0004
B (catalyst)	75.00	1	75.00	18.12	0.0053
AB	8.33	1	8.33	2.01	0.2060
Error	24.84	6	4.14		
Total	323.00	11			

would be made in random order. The analysis of the design is similar to that of any blocked factorial experiment; for example, see the discussion in Section 5-6.

EXAMPLE 7-1

Consider the chemical process experiment first described in Section 6-2. Suppose that only four experimental trials can be made from a single batch of raw material. Therefore, three batches of raw material will be required to run all three replicates of this design. Table 7-1 (on the previous page) shows the design, where each batch of raw material corresponds to a block.

The analysis of variance for this blocked design is shown in Table 7-2. All of the sums of squares are calculated exactly as in a standard, unblocked 2^k design. The sum of squares for blocks is calculated from the block totals. Let B_1, B_2, and B_3 represent the block totals (see Table 7-1). Then

$$\begin{aligned} SS_{\text{Blocks}} &= \sum_{i=1}^{3} \frac{B_i^2}{4} - \frac{y_{...}^2}{12} \\ &= \frac{(113)^2 + (106)^2 + (111)^2}{4} - \frac{(330)^2}{12} \\ &= 6.50 \end{aligned}$$

There are two degrees of freedom among the three blocks. Table 7-2 indicates that the conclusions from this analysis, had the design been run in blocks, are identical to those in Section 6-2 and that the block effect is relatively small.

7-3 CONFOUNDING IN THE 2^k FACTORIAL DESIGN

There are many problems for which it is impossible to perform a complete replicate of a factorial design in one block. **Confounding** is a design technique for arranging a complete factorial experiment in blocks, where the block size is smaller than the number of treatment combinations in one replicate. The technique causes information about certain treatment effects (usually high-order interactions) to be **indistinguishable from**, or **confounded with**, **blocks**. In this chapter we concentrate on confounding systems for the 2^k factorial design. Note that even though the designs presented are incomplete block designs because each block does not contain all the treatments or treatment combinations, the special structure of the 2^k factorial system allows a simplified method of analysis.

We consider the construction and analysis of the 2^k factorial design in 2^p incomplete blocks, where $p < k$. Consequently, these designs can be run in two blocks, four blocks, eight blocks, and so on.

7-4 CONFOUNDING THE 2^k FACTORIAL DESIGN IN TWO BLOCKS

Suppose that we wish to run a single replicate of the 2^2 design. Each of the $2^2 = 4$ treatment combinations requires a quantity of raw material, for example, and each batch of raw material is only large enough for two treatment combinations to be tested. Thus, two batches of raw material are required. If batches of raw material are considered as blocks, then we must assign two of the four treatment combinations to each block.

Figure 7-1 shows one possible design for this problem. The geometric view, Figure 7-1*a*, indicates that treatment combinations on opposing diagonals are assigned to different blocks. Notice from Figure 7-1*b* that block 1 contains the treatment combinations (1) and *ab* and that block 2 contains *a* and *b*. Of course, the *order* in which the treatment combinations are run within a block is randomly determined. We would also randomly decide which block to run first. Suppose we estimate the main effects of *A* and *B* just as if no blocking had occurred. From Equations 6-1 and 6-2, we obtain

$$A = \tfrac{1}{2}[ab + a - b - (1)]$$

$$B = \tfrac{1}{2}[ab + b - a - (1)]$$

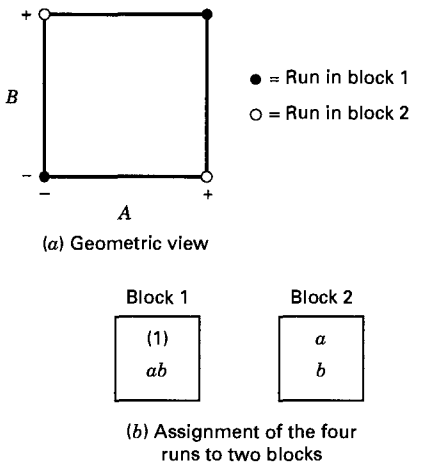
Note that both *A* and *B* are unaffected by blocking because in each estimate there is one plus and one minus treatment combination from each block. That is, any difference between block 1 and block 2 will cancel out.

Now consider the *AB* interaction

$$AB = \tfrac{1}{2}[ab + (1) - a - b]$$

Because the two treatment combinations with the plus sign [*ab* and (1)] are in block 1 and the two with the minus sign (*a* and *b*) are in block 2, the block effect and the *AB* interaction are identical. That is, *AB* is **confounded** with blocks.

The reason for this is apparent from the table of plus and minus signs for the 2^2 design. This was originally given as Table 6-2, but for convenience it is reproduced as Table 7-3 on the next page. From this table, we see that all treatment combinations that have a plus sign on *AB* are assigned to block 1, whereas all treatment combinations that



(*a*) Geometric view

(*b*) Assignment of the four runs to two blocks

Figure 7-1 A 2^2 design in two blocks.

Table 7-3 Table of Plus and Minus Signs for the 2^2 Design

Treatment Combination	Factorial Effect			
	I	A	B	AB
(1)	+	−	−	+
a	+	+	−	−
b	+	−	+	−
ab	+	+	+	+

have a minus sign on AB are assigned to block 2. This approach can be used to confound any effect (A, B, or AB) with blocks. For example, if (1) and b had been assigned to block 1 and a and ab to block 2, the main effect A would have been confounded with blocks. The usual practice is to confound the highest-order interaction with blocks.

This scheme can be used to confound any 2^k design in two blocks. As a second example, consider a 2^3 design run in two blocks. Suppose we wish to confound the three-factor interaction ABC with blocks. From the table of plus and minus signs shown in Table 7-4, we assign the treatment combinations that are minus on ABC to block 1 and those that are plus on ABC to block 2. The resulting design is shown in Figure 7-2. Once again, we emphasize that the treatment combinations *within* a block are run in random order.

Other Methods for Constructing the Blocks

There is another method for constructing these designs. The method uses the linear combination

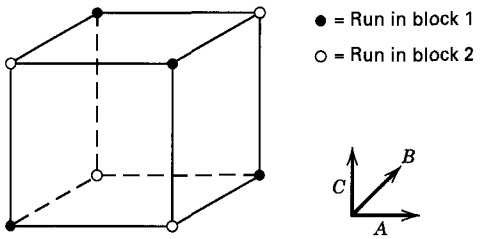
$$L = \alpha_1 x_1 + \alpha_2 x_2 + \cdots + \alpha_k x_k \tag{7-1}$$

where x_i is the level of the ith factor appearing in a particular treatment combination and α_i is the exponent appearing on the ith factor in the effect to be confounded. For the 2^k system, we have $\alpha_i = 0$ or 1 and $x_i = 0$ (low level) or $x_i = 1$ (high level). Equation 7-1 is called a **defining contrast**. Treatment combinations that produce the same value of L (mod 2) will be placed in the same block. Because the only possible values of L (mod 2) are 0 and 1, this will assign the 2^k treatment combinations to exactly two blocks.

To illustrate the approach, consider a 2^3 design with ABC confounded with blocks.

Table 7-4 Table of Plus and Minus Signs for the 2^3 Design

Treatment Combination	Factorial Effect							
	I	A	B	AB	C	AC	BC	ABC
(1)	+	−	−	+	−	+	+	−
a	+	+	−	−	−	−	+	+
b	+	−	+	−	−	+	−	+
ab	+	+	+	+	−	−	−	−
c	+	−	−	+	+	−	−	+
ac	+	+	−	−	+	+	−	−
bc	+	−	+	−	+	−	+	−
abc	+	+	+	+	+	+	+	+



(a) Geometric view

Block 1	Block 2
(1)	a
ab	b
ac	c
bc	abc

(b) Assignment of the eight runs to two blocks

Figure 7-2 The 2^3 design in two blocks with ABC confounded.

Here x_1 corresponds to A, x_2 to B, x_3 to C, and $\alpha_1 = \alpha_2 = \alpha_3 = 1$. Thus, the defining contrast corresponding to ABC is

$$L = x_1 + x_2 + x_3$$

The treatment combination (1) is written 000 in the (0, 1) notation; therefore,

$$L = 1(0) + 1(0) + 1(0) = 0 = 0 \pmod 2$$

Similarly, the treatment combination a is 100, yielding

$$L = 1(1) + 1(0) + 1(0) = 1 = 1 \pmod 2$$

Thus, (1) and a would be run in different blocks. For the remaining treatment combinations, we have

$$\begin{aligned}
b:&\quad L = 1(0) + 1(1) + 1(0) = 1 = 1 \pmod 2\\
ab:&\quad L = 1(1) + 1(1) + 1(0) = 2 = 0 \pmod 2\\
c:&\quad L = 1(0) + 1(0) + 1(1) = 1 = 1 \pmod 2\\
ac:&\quad L = 1(1) + 1(0) + 1(1) = 2 = 0 \pmod 2\\
bc:&\quad L = 1(0) + 1(1) + 1(1) = 2 = 0 \pmod 2\\
abc:&\quad L = 1(1) + 1(1) + 1(1) = 3 = 1 \pmod 2
\end{aligned}$$

Thus (1), ab, ac, and bc are run in block 1 and a, b, c, and abc are run in block 2. This is the same design shown in Figure 7-2, which was generated from the table of plus and minus signs.

Another method may be used to construct these designs. The block containing the treatment combination (1) is called the **principal block**. The treatment combinations in this block have a useful group-theoretic property; namely, they form a group with respect to multiplication modulus 2. This implies that any element [except (1)] in the principal

block may be generated by multiplying two other elements in the principal block modulus 2. For example, consider the principal block of the 2^3 design with ABC confounded, as shown in Figure 7-2. Note that

$$ab \cdot ac = a^2bc = bc$$
$$ab \cdot bc = ab^2c = ac$$
$$ac \cdot bc = abc^2 = ab$$

Treatment combinations in the other block (or blocks) may be generated by multiplying one element in the new block by each element in the principal block modulus 2. For the 2^3 with ABC confounded, because the principal block is (1), ab, ac, and bc, we know that b is in the other block. Thus, the elements of this second block are

$$b \cdot (1) = b$$
$$b \cdot ab = ab^2 = a$$
$$b \cdot ac = abc$$
$$b \cdot bc = b^2c = c$$

This agrees with the results obtained previously.

Estimation of Error

When the number of variables is small, say $k = 2$ or 3, it is usually necessary to replicate the experiment to obtain an estimate of error. For example, suppose that a 2^3 factorial must be run in two blocks with ABC confounded, and the experimenter decides to replicate the design four times. The resulting design might appear as in Figure 7-3. Note that ABC is confounded in each replicate.

The analysis of variance for this design is shown in Table 7-5. There are 32 observations and 31 total degrees of freedom. Furthermore, because there are eight blocks, seven degrees of freedom must be associated with these blocks. One breakdown of those seven degrees of freedom is shown in Table 7-5. The error sum of squares actually consists of the two-factor interactions between replicates and each of the effects (A, B, C, AB, AC, BC). It is usually safe to consider the interactions to be zero and to treat the resulting mean square as an estimate of error. Main effects and two-factor interactions are tested against the mean square error. Cochran and Cox (1957) observe that the block or ABC mean square could be compared to the error for the ABC mean square, which is really replicates $\times$ blocks. This test usually is very insensitive.

If resources are sufficient to allow the replication of confounded designs, it is generally better to use a slightly different method of designing the blocks in each replicate. This approach consists of confounding a different effect in each replicate so that some

Replicate I		Replicate II		Replicate III		Replicate IV	
Block 1	Block 2	Block 1	Block 2	Block 1	Block 2	Block 1	Block 2
(1)	*abc*	(1)	*abc*	(1)	*abc*	(1)	*abc*
ac	*a*	*ac*	*a*	*ac*	*a*	*ac*	*a*
ab	*b*	*ab*	*b*	*ab*	*b*	*ab*	*b*
bc	*c*	*bc*	*c*	*bc*	*c*	*bc*	*c*

Figure 7-3 Four replicates of the 2^3 design with ABC confounded.

Table 7-5 Analysis of Variance for Four Replicates of a 2^3 Design with ABC Confounded

Source of Variation	Degrees of Freedom
Replicates	3
Blocks (ABC)	1
Error for ABC (replicates × blocks)	3
A	1
B	1
C	1
AB	1
AC	1
BC	1
Error (or replicates × effects)	18
Total	31

information on all effects is obtained. Such a procedure is called **partial confounding** and is discussed in Section 7-7. If k is moderately large, say $k \geq 4$, we frequently can afford only a single replicate. The experimenter usually assumes higher-order interactions to be negligible and combines their sums of squares as error. The normal probability plot of factor effects can be very helpful in this regard.

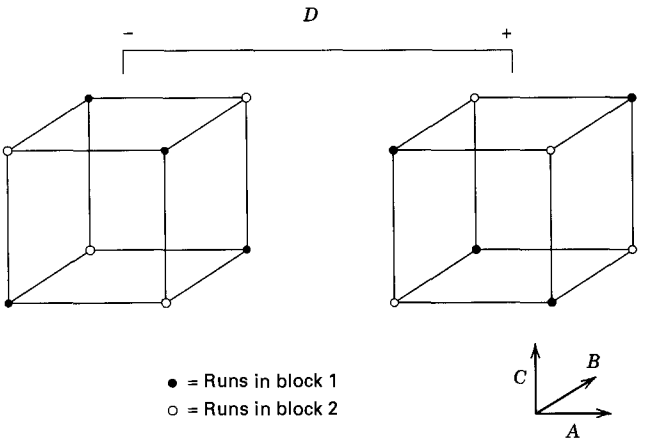
EXAMPLE 7-2

Consider the situation described in Example 6-2. Recall that four factors—temperature (A), pressure (B), concentration of formaldehyde (C), and stirring rate (D)—are studied in a pilot plant to determine their effect on product filtration rate. We will use this experiment to illustrate the ideas of blocking and confounding in an unreplicated design. We will make two modifications to the original experiment. First, suppose that the $2^4 = 16$ treatment combinations cannot all be run using one batch of raw material. The experimenter can run eight treatment combinations from a single batch of material, so a 2^4 design confounded in two blocks seems appropriate. It is logical to confound the highest-order interaction $ABCD$ with blocks. The defining contrast is

$$L = x_1 + x_2 + x_3 + x_4$$

and it is easy to verify that the design is as shown in Figure 7-4 (on the next page). Alternatively, one may examine Table 6-11 and observe that the treatment combinations that are + in the $ABCD$ column are assigned to block 1 and those that are − in $ABCD$ column are in block 2.

The second modification that we will make is to introduce a block effect so that the utility of blocking can be demonstrated. Suppose that when we select the two batches of raw material required to run the experiment, one of them is of much poorer quality and, as a result, all responses will be 20 units lower in this material batch than in the other. The poor quality batch becomes block 1 and the good quality batch becomes block 2 (it doesn't matter which batch is called block 1 or which batch is called block 2). Now all the tests in block 1 are performed first (the eight runs in the block are, of course, performed in random order), but the responses are 20 units lower than they would have been



(*a*) Geometric view

Block 1	Block 2
(1) = 25	*a* = 71
ab = 45	*b* = 48
ac = 40	*c* = 68
bc = 60	*d* = 43
ad = 80	*abc* = 65
bd = 25	*bcd* = 70
cd = 55	*acd* = 86
abcd = 76	*abd* = 104

(*b*) Assignment of the 16 runs to two blocks

Figure 7-4 The 2^4 design in two blocks for Example 7-2.

if good quality material had been used. Figure 7-4*b* shows the resulting responses—note that these have been found by subtracting the block effect from the original observations given in Example 6-2. That is, the original response for treatment combination (1) was 45, and in Figure 7-4*b* it is reported as (1) = 25 (= 45 − 20). The other responses in this block are obtained similarly. After the tests in block 1 are performed, the eight tests in block 2 follow. There is no problem with the raw material in this batch, so the responses are exactly as they were originally in Example 6-2.

The effect estimates for this "modified" version of Example 6-2 are shown in Table 7-6. Note that the estimates of the four main effects, the six two-factor interactions, and the four three-factor interactions are identical to the effect estimates obtained in Example 6-2 where there was *no block effect*. When a normal probability of these effect estimates is constructed, factors *A*, *C*, *D* and the *AC* and *AD* interactions emerge as the important effects, just as in the original experiment. (The reader should verify this.)

What about the *ABCD* interaction effect? The estimate of this effect in the original experiment (Example 6-2) was *ABCD* = 1.375. In the present example, the estimate of the *ABCD* interaction effect is *ABCD* = −18.625. Because *ABCD* is confounded with blocks, the *ABCD* interaction estimates the *original interaction effect* (1.375) plus the *block effect* (−20), so *ABCD* = 1.375 + (−20) = −18.625. (Do you see why the block

Table 7-6 Effect Estimates for the Blocked 2^4 Design in Example 7-2

Model Term	Regression Coefficient	Effect Estimate	Sum of Squares	Percent Contribution
A	10.81	21.625	1870.5625	26.30
B	1.56	3.125	39.0625	0.55
C	4.94	9.875	390.0625	5.49
D	7.31	14.625	855.5625	12.03
AB	0.062	0.125	0.0625	<0.01
AC	−9.06	−18.125	1314.0625	18.48
AD	8.31	16.625	1105.5625	15.55
BC	1.19	2.375	22.5625	0.32
BD	−0.19	−0.375	0.5625	<0.01
CD	−0.56	−1.125	5.0625	0.07
ABC	0.94	1.875	14.0625	0.20
ABD	2.06	4.125	68.0625	0.96
ACD	−0.81	−1.625	10.5625	0.15
BCD	−1.31	−2.625	27.5625	0.39
Blocks (*ABCD*)		−18.625	1387.5625	19.51

effect is −20?) The block effect may also be calculated directly as the difference in average response between the two blocks, or

$$\begin{aligned}\text{Block Effect} &= \bar{y}_{\text{Block 1}} - \bar{y}_{\text{Block 2}} \\ &= \frac{406}{8} - \frac{555}{8} \\ &= \frac{-149}{8} \\ &= -18.625\end{aligned}$$

Of course, this effect really estimates Blocks + *ABCD*.

Table 7-7 summarizes the analysis of variance for this experiment. The effects with large estimates are included in the model, and the block sum of squares is

$$SS_{\text{Blocks}} = \frac{(406)^2 + (555)^2}{8} - \frac{(961)^2}{16} = 1387.5625$$

Table 7-7 Analysis of Variance for Example 7-2

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	*P*-Value
Blocks (*ABCD*)	1387.5625	1			
A	1870.5625	1	1870.5625	89.76	<0.0001
C	390.0625	1	390.0625	18.72	0.0019
D	855.5625	1	855.5625	41.05	0.0001
AC	1314.0625	1	1314.0625	63.05	<0.0001
AD	1105.5625	1	1105.5625	53.05	<0.0001
Error	187.5625	9	20.8403		
Total	7111.4375	15			

The conclusions from this experiment exactly match those from Example 6-2, where no block effect was present. Notice that if the experiment had not been run in blocks, and if an effect of magnitude -20 had affected the first 8 trials (which would have been selected in a random fashion, because the 16 trials would be run in random order in an unblocked design), the results could have been very different.

7-5 CONFOUNDING THE 2^k FACTORIAL DESIGN IN FOUR BLOCKS

It is possible to construct 2^k factorial designs confounded in four blocks of 2^{k-2} observations each. These designs are particularly useful in situations where the number of factors is moderately large, say $k \geq 4$, and block sizes are relatively small.

As an example, consider the 2^5 design. If each block will hold only eight runs, then four blocks must be used. The construction of this design is relatively straightforward. Select *two* effects to be confounded with blocks, say *ADE* and *BCE*. These effects have the two defining contrasts

$$L_1 = x_1 + x_4 + x_5$$
$$L_2 = x_2 + x_3 + x_5$$

associated with them. Now every treatment combination will yield a particular pair of values of L_1 (mod 2) and L_2 (mod 2), that is, either $(L_1, L_2) = (0, 0)$, $(0, 1)$, $(1, 0)$, or $(1, 1)$. Treatment combinations yielding the same values of (L_1, L_2) are assigned to the same block. In our example we find

$L_1 = 0, L_2 = 0$	for	(1), *ad*, *bc*, *abcd*, *abe*, *ace*, *cde*, *bde*
$L_1 = 1, L_2 = 0$	for	*a*, *d*, *abc*, *bcd*, *be*, *abde*, *ce*, *acde*
$L_1 = 0, L_2 = 1$	for	*b*, *abd*, *c*, *acd*, *ae*, *de*, *abce*, *bcde*
$L_1 = 1, L_2 = 1$	for	*e*, *ade*, *bce*, *abcde*, *ab*, *bd*, *ac*, *cd*

These treatment combinations would be assigned to different blocks. The complete design is as shown in Figure 7-5.

With a little reflection we realize that another effect in addition to *ADE* and *BCE* must be confounded with blocks. Because there are four blocks with three degrees of freedom between them, and because *ADE* and *BCE* have only one degree of freedom each, clearly an additional effect with one degree of freedom must be confounded. This effect is the **generalized interaction** of *ADE* and *BCE*, which is defined as the product

Block 1	Block 2	Block 3	Block 4
$L_1 = 0$	$L_1 = 1$	$L_1 = 0$	$L_1 = 1$
$L_2 = 0$	$L_2 = 0$	$L_2 = 1$	$L_2 = 1$
(1) *abc*	*a be*	*b abce*	*e abcde*
ad ace	*d abde*	*abd ae*	*ade bd*
bc cde	*abc ce*	*c bcde*	*bce ac*
abcd bde	*bcd acde*	*acd de*	*ab cd*

Figure 7-5 The 2^5 design in four blocks with *ADE*, *BCE*, and *ABCD* confounded.

of ADE and BCE modulus 2. Thus, in our example the generalized interaction $(ADE)(BCE) = ABCDE^2 = ABCD$ is also confounded with blocks. It is easy to verify this by referring to a table of plus and minus signs for the 2^5 design, such as in Davies (1956). Inspection of such a table reveals that the treatment combinations are assigned to the blocks as follows:

Treatment Combinations in	Sign on ADE	Sign on BCE	Sign on $ABCD$
Block 1	−	−	+
Block 2	+	−	−
Block 3	−	+	−
Block 4	+	+	+

Notice that the product of signs of any two effects for a particular block (e.g., ADE and BCE) yields the sign of the other effect for that block (in this case, $ABCD$). Thus, ADE, BCE, and $ABCD$ are all confounded with blocks.

The group-theoretic properties of the principal block mentioned in Section 7-4 still hold. For example, we see that the product of two treatment combinations in the principal block yields another element of the principal block. That is,

$$ad \cdot bc = abcd \qquad \text{and} \qquad abe \cdot bde = ab^2de^2 = ad$$

and so forth. To construct another block, select a treatment combination that is not in the principal block (e.g., b) and multiply b by all the treatment combinations in the principal block. This yields

$$b \cdot (1) = b \qquad b \cdot ad = abd \qquad b \cdot bc = b^2c = c \qquad b \cdot abcd = ab^2cd = acd$$

and so forth, which will produce the eight treatment combinations in block 3. In practice, the principal block can be obtained from the defining contrasts and the group-theoretic property, and the remaining blocks can be determined from these treatment combinations by the method shown above.

The general procedure for constructing a 2^k design confounded in four blocks is to choose two effects to generate the blocks, automatically confounding a third effect that is the generalized interaction of the first two. Then, the design is constructed by using the two defining contrasts (L_1, L_2) and the group-theoretic properties of the principal block. In selecting effects to be confounded with blocks, care must be exercised to obtain a design that does not confound effects that may be of interest. For example, in a 2^5 design we might choose to confound $ABCDE$ and ABD, which automatically confounds CE, an effect that is probably of interest. A better choice is to confound ADE and BCE, which automatically confounds $ABCD$. It is preferable to sacrifice information on the three-factor interactions ADE and BCE instead of the two-factor interaction CE.

7-6 CONFOUNDING THE 2^k FACTORIAL DESIGN IN 2^p BLOCKS

The methods described above may be extended to the construction of a 2^k factorial design confounded in 2^p blocks $(p < k)$, where each block contains exactly 2^{k-p} runs. We select p independent effects to be confounded, where by "independent" we mean that no effect chosen is the generalized interaction of the others. The blocks may be generated by use

Table 7-8 Suggested Blocking Arrangements for the 2^k Factorial Design

Number of Factors, k	Number of Blocks, 2^p	Block Size, 2^{k-p}	Effects Chosen to Generate the Blocks	Interactions Confounded with Blocks
3	2	4	*ABC*	*ABC*
	4	2	*AB*, *AC*	*AB*, *AC*, *BC*
4	2	8	*ABCD*	*ABCD*
	4	4	*ABC*, *ACD*	*ABC*, *ACD*, *BD*
	8	2	*AB*, *BC*, *CD*	*AB*, *BC*, *CD*, *AC*, *BD*, *AD*, *ABCD*
5	2	16	*ABCDE*	*ABCDE*
	4	8	*ABC*, *CDE*	*ABC*, *CDE*, *ABDE*
	8	4	*ABE*, *BCE*, *CDE*	*ABE*, *BCE*, *CDE*, *AC*, *ABCD*, *BD*, *ADE*
	16	2	*AB*, *AC*, *CD*, *DE*	All two- and four-factor interactions (15 effects)
6	2	32	*ABCDEF*	*ABCDEF*
	4	16	*ABCF*, *CDEF*	*ABCF*, *CDEF*, *ABDE*
	8	8	*ABEF*, *ABCD*, *ACE*	*ABEF*, *ABCD*, *ACE*, *BCF*, *BDE*, *CDEF*, *ADF*
	16	4	*ABF*, *ACF*, *BDF*, *DEF*	*ABE*, *ACF*, *BDF*, *DEF*, *BC*, *ABCD*, *ABDE*, *AD*, *ACDE*, *CE*, *BDF*, *BCDEF*, *ABCEF*, *AEF*, *BE*
	32	2	*AB*, *BC*, *CD*, *DE*, *EF*	All two-, four-, and six-factor interactions (31 effects)
7	2	64	*ABCDEFG*	*ABCDEFG*
	4	32	*ABCFG*, *CDEFG*	*ABCFG*, *CDEFG*, *ABDE*
	8	16	*ABC*, *DEF*, *AFG*	*ABC*, *DEF*, *AFG*, *ABCDEF*, *BCFG*, *ADEG*, *BCDEG*
	16	8	*ABCD*, *EFG*, *CDE*, *ADG*	*ABCD*, *EFG*, *CDE*, *ADG*, *ABCDEFG*, *ABE*, *BCG*, *CDFG*, *ADEF*, *ACEG*, *ABFG*, *BCEF*, *BDEG*, *ACF*, *BDF*
	32	4	*ABG*, *BCG*, *CDG*, *DEG*, *EFG*	*ABG*, *BCG*, *CDG*, *DEG*, *EFG*, *AC*, *BD*, *CE*, *DF*, *AE*, *BE*, *ABCD*, *ABDE*, *ABEF*, *BCDE*, *BCEF*, *CDEF*, *ABCDEFG*, *ADG*, *ACDEG*, *ACEFG*, *ABDFG*, *ABCEG*, *BEG*, *BDEFG*, *CFG*, *ADEF*, *ACDF*, *ABCF*, *AFG*
	64	2	*AB*, *BC*, *CD*, *DE*, *EF*, *FG*	All two-, four-, and six-factor interactions (63 effects)

of the p defining contrasts $L_1, L_2, \ldots, L_p$ associated with these effects. In addition, exactly $2^p - p - 1$ other effects will be confounded with blocks, these being the generalized interactions of those p independent effects initially chosen. Care should be exercised in selecting effects to be confounded so that information on effects that may be of potential interest is not sacrificed.

The statistical analysis of these designs is straightforward. Sums of squares for all the effects are computed as if no blocking had occurred. Then, the block sum of squares is found by adding the sums of squares for all the effects confounded with blocks.

Obviously, the choice of the p effects used to generate the block is critical because the confounding structure of the design directly depends on them. Table 7-8 (on the facing page) presents a list of useful designs. To illustrate the use of this table, suppose we wish to construct a 2^6 design confounded in $2^3 = 8$ blocks of $2^3 = 8$ runs each. Table 7-8 indicates that we would choose $ABEF$, $ABCD$, and ACE as the $p = 3$ independent effects to generate the blocks. The remaining $2^p - p - 1 = 2^3 - 3 - 1 = 4$ effects that are confounded are the generalized interactions of these three; that is,

$$\begin{aligned}(ABEF)(ABCD) &= A^2B^2CDEF = CDEF\\ (ABEF)(ACE) &= A^2BCE^2F = BCF\\ (ABCD)(ACE) &= A^2BC^2ED = BDE\\ (ABEF)(ABCD)(ACE) &= A^3B^2C^2DE^2F = ADF\end{aligned}$$

The reader is asked to generate the eight blocks for this design in Problem 7-11.

7-7 PARTIAL CONFOUNDING

We remarked in Section 7-4 that, unless experimenters have a prior estimate of error or are willing to assume certain interactions to be negligible, they must replicate the design to obtain an estimate of error. Figure 7-3 shows a 2^3 factorial in two blocks with ABC confounded, replicated four times. From the analysis of variance for this design, shown in Table 7-5, we note that information on the ABC interaction cannot be retrieved because ABC is confounded with blocks *in each replicate*. This design is said to be **completely confounded**.

Consider the alternative shown in Figure 7-6. Once again, there are four replicates of the 2^3 design, but a *different* interaction has been confounded in each replicate. That is, ABC is confounded in replicate I, AB is confounded in replicate II, BC is confounded in replicate III, and AC is confounded in replicate IV. As a result, information on ABC

Replicate I		Replicate II		Replicate III		Replicate IV	
ABC Confounded		*AB* Confounded		*BC* Confounded		*AC* Confounded	
(1)	*a*	(1)	*a*	(1)	*b*	(1)	*a*
ab	*b*	*c*	*b*	*a*	*c*	*b*	*c*
ac	*c*	*ab*	*ac*	*bc*	*ab*	*ac*	*ab*
bc	*abc*	*abc*	*bc*	*abc*	*ac*	*abc*	*bc*

Figure 7-6 Partial confounding in the 2^3 design.

Table 7-9 Analysis of Variance for a Partially Confounded 2^3 Design

Source of Variation	Degrees of Freedom
Replicates	3
Blocks within replicates [or *ABC* (rep. I) + *AB* (rep. II) + *BC* (rep. III) + *AC* (rep. IV)]	4
A	1
B	1
C	1
AB (from replicates I, III, and IV)	1
AC (from replicates I, II, and III)	1
BC (from replicates I, II, and IV)	1
ABC (from replicates II, III, and IV)	1
Error	17
Total	31

can be obtained from the data in replicates II, III, and IV; information on *AB* can be obtained from replicates I, III, and IV; information on *AC* can be obtained from replicates I, II, and III; and information on *BC* can be obtained from replicates I, II, and IV. We say that three-quarters information can be obtained on the interactions because they are unconfounded in only three replicates. Yates (1937) calls the ratio 3/4 the **relative information for the confounded effects**. This design is said to be **partially confounded**.

The analysis of variance for this design is shown in Table 7-9. In calculating the interaction sums of squares, only data from the replicates in which an interaction is unconfounded are used. The error sum of squares consists of replicates × main effect sums of squares plus replicates × interaction sums of squares for each replicate in which that interaction is unconfounded (e.g., replicates × *ABC* for replicates II, III, and IV). Furthermore, there are seven degrees of freedom among the eight blocks. This is usually partitioned into three degrees of freedom for replicates and four degrees of freedom for blocks within replicates. The composition of the sum of squares for blocks is shown in Table 7-9 and follows directly from the choice of the effect confounded in each replicate.

EXAMPLE 7-3

A 2^3 Design with Partial Confounding

Consider Example 6-1, in which a study was performed to determine the effect of percentage of carbonation (*A*), operating pressure (*B*), and line speed (*C*) on the fill height of a carbonated beverage. Suppose that each batch of syrup is only large enough to test four treatment combinations. Thus, each replicate of the 2^3 design must be run in two blocks. Two replicates are run, with *ABC* confounded in replicate I and *AB* confounded in replicate II. The data are as follows:

Replicate I, *ABC* Confounded		Replicate II, *AB* Confounded	
(1) = −3	*a* = 0	(1) = −1	*a* = 1
ab = 2	*b* = −1	*c* = 0	*b* = 0
ac = 2	*c* = −1	*ab* = 3	*ac* = 1
bc = 1	*abc* = 6	*abc* = 5	*bc* = 1

Table 7-10 Analysis of Variance for Example 7-3

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Replicates	1.00	1	1.00	—	
Blocks within replicates	2.50	2	1.25	—	
A	36.00	1	36.00	48.00	0.0001
B	20.25	1	20.25	27.00	0.0035
C	12.25	1	12.25	16.33	0.0099
AB (rep. I only)	0.50	1	0.50	0.67	0.4503
AC	0.25	1	0.25	0.33	0.5905
BC	1.00	1	1.00	1.33	0.3009
ABC (rep. II only)	0.50	1	0.50	0.67	0.4503
Error	3.75	5	0.75	—	
Total	78.00	15	—	—	

The sums of squares for A, B, C, AC, and BC may be calculated in the usual manner, using all 16 observations. However, we must find SS_{ABC} using only the data in replicate II and SS_{AB} using only the data in replicate I as follows:

$$SS_{ABC} = \frac{[a + b + c + abc - ab - ac - bc - (1)]^2}{n2^k}$$
$$= \frac{[1 + 0 + 0 + 5 - 3 - 1 - 1 - (-1)]^2}{(1)(8)} = 0.50$$
$$S_{AB} = \frac{[(1) + abc - ac + c - a - b + ab - bc]^2}{n2^k}$$
$$= \frac{[-3 + 6 - 2 + (-1) - 0 - (-1) + 2 - 1]^2}{(1)(8)} = 0.50$$

The sum of squares for the replicates is, in general,

$$SS_{\text{Rep}} = \sum_{h=1}^{n} \frac{R_h^2}{2^k} - \frac{y_{...}^2}{N}$$
$$= \frac{(6)^2 + (10)^2}{8} - \frac{(16)^2}{16} = 1.00$$

where R_h is the total of the observations in the hth replicate. The block sum of squares is the sum of SS_{ABC} from replicate I and SS_{AB} from replicate II, or $SS_{\text{Blocks}} = 2.50$.

The analysis of variance is summarized in Table 7-10. All three main effects are important.

7-8 PROBLEMS

7-1. Consider the experiment described in Problem 6-1. Analyze this experiment assuming that each replicate represents a block of a single production shift.

7-2. Consider the experiment described in Problem 6-5. Analyze this experiment assuming that each one of the four replicates represents a block.

7-3. Consider the alloy cracking experiment described in Problem 6-15. Suppose that only 16 runs could be made on a single day, so each replicate was treated as a block. Analyze the experiment and draw conclusions.

7-4. Consider the data from the first replicate of Problem 6-1. Suppose that these observations could not all be run using the same bar stock. Set up a design to run these observations in two blocks of four observations each with *ABC* confounded. Analyze the data.

7-5. Consider the data from the first replicate of Problem 6-7. Construct a design with two blocks of eight observations each with *ABCD* confounded. Analyze the data.

7-6. Repeat Problem 7-5 assuming that four blocks are required. Confound *ABD* and *ABC* (and consequently *CD*) with blocks.

7-7. Using the data from the 2^5 design in Problem 6-21, construct and analyze a design in two blocks with *ABCDE* confounded with blocks.

7-8. Repeat Problem 7-7 assuming that four blocks are necessary. Suggest a reasonable confounding scheme.

7-9. Consider the data from the 2^5 design in Problem 6-21. Suppose that it was necessary to run this design in four blocks with *ACDE* and *BCD* (and consequently *ABE*) confounded. Analyze the data from this design.

7-10. Design an experiment for confounding a 2^6 factorial in four blocks. Suggest an appropriate confounding scheme, different from the one shown in Table 7-8.

7-11. Consider the 2^6 design in eight blocks of eight runs each with *ABCD*, *ACE*, and *ABEF* as the independent effects chosen to be confounded with blocks. Generate the design. Find the other effects confounded with blocks.

7-12. Consider the 2^2 design in two blocks with *AB* confounded. Prove algebraically that $SS_{AB} = SS_{\text{Blocks}}$.

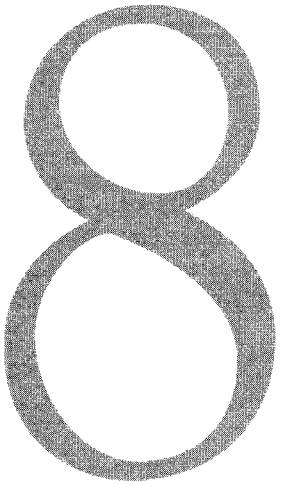
7-13. Consider the data in Example 7-2. Suppose that all the observations in block 2 are increased by 20. Analyze the data that would result. Estimate the block effect. Can you explain its magnitude? Do blocks now appear to be an important factor? Are any other effect estimates impacted by the change you made to the data?

7-14 Suppose that in Problem 6-1 we had confounded *ABC* in replicate I, *AB* in replicate II, and *BC* in replicate III. Calculate the factor effect estimates. Construct the analysis of variance table.

7-15. Repeat Problem 6-1 assuming that *ABC* was confounded with blocks in each replicate.

7-16. Suppose that in Problem 6-7 *ABCD* was confounded in replicate I and *ABC* was confounded in replicate II. Perform the statistical analysis of this design.

7-17. Construct a 2^3 design with *ABC* confounded in the first two replicates and *BC* confounded in the third. Outline the analysis of variance and comment on the information obtained.



Two-Level Fractional Factorial Designs

8-1 INTRODUCTION

As the number of factors in a 2^k factorial design increases, the number of runs required for a complete replicate of the design rapidly outgrows the resources of most experimenters. For example, a complete replicate of the 2^6 design requires 64 runs. In this design only 6 of the 63 degrees of freedom correspond to main effects, and only 15 degrees of freedom correspond to two-factor interactions. The remaining 42 degrees of freedom are associated with three-factor and higher interactions.

If the experimenter can reasonably assume that certain high-order interactions are negligible, information on the main effects and low-order interactions may be obtained by running only a fraction of the complete factorial experiment. These **fractional factorial designs** are among the most widely used types of designs for product and process design and for process improvement.

A major use of fractional factorials is in **screening experiments**. These are experiments in which many factors are considered and the objective is to identify those factors (if any) that have large effects. Screening experiments are usually performed in the early stages of a project when it is likely that many of the factors initially considered have little or no effect on the response. The factors that are identified as important are then investigated more thoroughly in subsequent experiments.

The successful use of fractional factorial designs is based on three key ideas:

1. ***The sparsity of effects principle.*** When there are several variables, the system or process is likely to be driven primarily by some of the main effects and low-order interactions.
2. ***The projection property.*** Fractional factorial designs can be projected into stronger (larger) designs in the subset of significant factors.
3. ***Sequential experimentation.*** It is possible to combine the runs of two (or more) fractional factorials to assemble sequentially a larger design to estimate the factor effects and interactions of interest.

We will focus on these principles in this chapter and illustrate them with several examples.

8-2 THE ONE-HALF FRACTION OF THE 2^k DESIGN

Consider a situation in which three factors, each at two levels, are of interest, but the experimenters cannot afford to run all $2^3 = 8$ treatment combinations. They can, however, afford four runs. This suggests a one-half fraction of a 2^3 design. Because the design contains $2^{3-1} = 4$ treatment combinations, a one-half fraction of the 2^3 design is often called a $\mathbf{2^{3-1}}$ **design.**

The table of plus and minus signs for the 2^3 design is shown in Table 8-1. Suppose we select the four treatment combinations a, b, c, and abc as our one-half fraction. These runs are shown in the top half of Table 8-1 and in Figure 8-1*a*.

Notice that the 2^{3-1} design is formed by selecting only those treatment combinations that have a plus in the ABC column. Thus, ABC is called the **generator** of this particular fraction. Sometimes we will refer to a generator such as ABC as a **word.** Furthermore, the identity column I is also always plus, so we call

$$I = ABC$$

the **defining relation** for our design. In general, the defining relation for a fractional factorial will always be the set of all columns that are equal to the identity column I.

The treatment combinations in the 2^{3-1} design yield three degrees of freedom that we may use to estimate the main effects. Referring to Table 8-1, we note that the linear combinations of the observations used to estimate the main effects of A, B, and C are

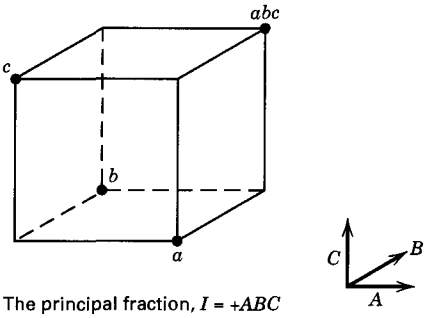
$$\ell_A = \tfrac{1}{2}(a - b - c + abc)$$
$$\ell_B = \tfrac{1}{2}(-a + b - c + abc)$$
$$\ell_C = \tfrac{1}{2}(-a - b + c + abc)$$

It is also easy to verify that the linear combinations of the observations used to estimate the two-factor interactions are

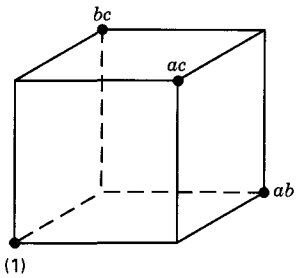
$$\ell_{BC} = \tfrac{1}{2}(a - b - c + abc)$$
$$\ell_{AC} = \tfrac{1}{2}(-a + b - c + abc)$$
$$\ell_{AB} = \tfrac{1}{2}(-a - b + c + abc)$$

Table 8-1 Plus and Minus Signs for the 2^3 Factorial Design

Treatment Combination	Factorial Effect							
	I	A	B	C	AB	AC	BC	ABC
a	+	+	−	−	−	−	+	+
b	+	−	+	−	−	+	−	+
c	+	−	−	+	+	−	−	+
abc	+	+	+	+	+	+	+	+
ab	+	+	+	−	+	−	−	−
ac	+	+	−	+	−	+	−	−
bc	+	−	+	+	−	−	+	−
(1)	+	−	−	−	+	+	+	−



(a) The principal fraction, $I = +ABC$



(b) The alternate fraction, $I = -ABC$

Figure 8-1 The two one-half fractions of the 2^3 design.

Thus, $\ell_A = \ell_{BC}$, $\ell_B = \ell_{AC}$, and $\ell_C = \ell_{AB}$; consequently, it is impossible to differentiate between A and BC, B and AC, and C and AB. In fact, when we estimate A, B, and C we are *really* estimating $A + BC$, $B + AC$, and $C + AB$. Two or more effects that have this property are called **aliases**. In our example, A and BC are aliases, B and AC are aliases, and C and AB are aliases. We indicate this by the notation $\ell_A \rightarrow A + BC$, $\ell_B \rightarrow B + AC$, and $\ell_C \rightarrow C + AB$.

The alias structure for this design may be easily determined by using the defining relation $I = ABC$. Multiplying any column (or effect) by the defining relation yields the aliases for that column (or effect). In our example, this yields as the alias of A

$$A \cdot I = A \cdot ABC = A^2BC$$

or, because the square of any column is just the identity I,

$$A = BC$$

Similarly, we find the aliases of B and C as

$$B \cdot I = B \cdot ABC$$
$$B = AB^2C = AC$$

and

$$C \cdot I = C \cdot ABC$$
$$C = ABC^2 = AB$$

This one-half fraction, with $I = +ABC$, is usually called the **principal fraction**.

Now suppose that we had chosen the *other* one-half fraction, that is, the treatment combinations in Table 8-1 associated with minus in the ABC column. This **alternate**, or

complementary, one-half fraction (consisting of the runs (1), *ab*, *ac*, and *bc*) is shown in Figure 8-1*b*. The defining relation for this design is

$$I = -ABC$$

The linear combination of the observations, say ℓ'_A, ℓ'_B, and ℓ'_C, from the alternate fraction gives us

$$\ell'_A \rightarrow A - BC$$
$$\ell'_B \rightarrow B - AC$$
$$\ell'_C \rightarrow C - AB$$

Thus, when we estimate A, B, and C with this particular fraction, we are really estimating $A - BC$, $B - AC$, and $C - AB$.

In practice, it does not matter which fraction is actually used. Both fractions belong to the same **family**; that is, the two one-half fractions form a complete 2^3 design. This is easily seen by reference to parts *a* and *b* of Figure 8-1.

Suppose that after running one of the one-half fractions of the 2^3 design, the other one was also run. Thus, all eight runs associated with the full 2^3 are now available. We may now obtain de-aliased estimates of all the effects by analyzing the eight runs as a full 2^3 design in two blocks of four runs each. This could also be done by adding and subtracting the linear combination of effects from the two individual fractions. For example, consider $\ell_A \rightarrow A + BC$ and $\ell'_A \rightarrow A - BC$. This implies that

$$\tfrac{1}{2}(\ell_A + \ell'_A) = \tfrac{1}{2}(A + BC + A - BC) \rightarrow A$$

and that

$$\tfrac{1}{2}(\ell_A - \ell'_A) = \tfrac{1}{2}(A + BC - A + BC) \rightarrow BC$$

Thus, for all three pairs of linear combinations, we would obtain the following:

i	From $\frac{1}{2}(\ell_i + \ell'_i)$	From $\frac{1}{2}(\ell_i - \ell'_i)$
A	A	BC
B	B	AC
C	C	AB

Design Resolution

The preceding 2^{3-1} design is called a **resolution III design**. In such a design, main effects are aliased with two-factor interactions. A design is of resolution R if no p-factor effect is aliased with another effect containing less than $R - p$ factors. We usually employ a Roman numeral subscript to denote design resolution; thus, the one-half fraction of the 2^3 design with the defining relation $I = ABC$ (or $I = -ABC$) is a 2^{3-1}_{III} design.

Designs of resolution III, IV, and V are particularly important. The definitions of these designs and an example of each follow:

1. ***Resolution III designs.*** These are designs in which no main effects are aliased with any other main effect, but main effects are aliased with two-factor interactions and two-factor interactions may be aliased with each other. The 2^{3-1} design in Table 8-1 is of resolution III (2^{3-1}_{III}).
2. ***Resolution IV designs.*** These are designs in which no main effect is aliased with any other main effect *or* with any two-factor interaction, but two-factor

interactions are aliased with each other. A 2^{4-1} design with $I = ABCD$ is a resolution IV design (2_{IV}^{4-1}).

3. ***Resolution V designs.*** These are designs in which no main effect or two-factor interaction is aliased with any other main effect or two-factor interaction, but two-factor interactions are aliased with three-factor interactions. A 2^{5-1} design with $I = ABCDE$ is a resolution V design (2_{V}^{5-1}).

In general, the resolution of a two-level fractional factorial design is equal to the smallest number of letters in any word in the defining relation. Consequently, we could call the preceding design types three-, four-, and five-letter designs, respectively. We usually like to employ fractional designs that have the highest possible resolution consistent with the degree of fractionation required. The higher the resolution, the less restrictive the assumptions that are required regarding which interactions are negligible to obtain a unique interpretation of the data.

Constructing One-Half Fractions

A one-half fraction of the 2^k design of the highest resolution may be constructed by writing down a **basic design** consisting of the runs for a *full* 2^{k-1} factorial and then adding the kth factor by identifying its plus and minus levels with the plus and minus signs of the highest-order interaction $ABC \cdots (K-1)$. Therefore, the 2_{III}^{3-1} fractional factorial is obtained by writing down the full 2^2 factorial as the basic design and then equating factor C to the AB interaction. The alternate fraction would be obtained by equating factor C to the $-AB$ interaction. This approach is illustrated in Table 8-2. Notice that the basic design always has the right number of runs (rows), but it is missing one column. The generator $I = ABC \cdots K$ is then solved for the missing column (K) so that $K = ABC \cdots (K-1)$ defines the product of plus and minus signs to use in each row to produce the levels for the kth factor.

Note that *any* interaction effect could be used to generate the column for the kth factor. However, using any effect other than $ABC \cdots (K-1)$ will not produce a design of the highest possible resolution.

Another way to view the construction of a one-half fraction is to partition the runs into two blocks with the highest-order interaction $ABC \cdots K$ confounded. Each block is a 2^{k-1} fractional factorial design of the highest resolution.

Projection of Fractions into Factorials

Any fractional factorial design of resolution R contains complete factorial designs (possibly replicated factorials) in any subset of $R-1$ factors. This is an important and useful concept. For example, if an experimenter has several factors of potential interest but

Table 8-2 The Two One-Half Fractions of the 2^3 Design

	Full 2^2 Factorial (Basic Design)		$2_{III}^{3-1}, I = ABC$			$2_{III}^{3-1}, I = -ABC$		
Run	A	B	A	B	$C = AB$	A	B	$C = -AB$
1	−	−	−	−	+	−	−	−
2	+	−	+	−	−	+	−	+
3	−	+	−	+	−	−	+	+
4	+	+	+	+	+	+	+	−

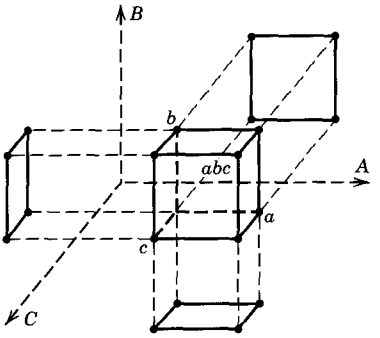


Figure 8-2 Projection of a 2^{3-1}_{III} design into three 2^2 designs.

believes that only $R - 1$ of them have important effects, then a fractional factorial design of resolution R is the appropriate choice of design. If the experimenter is correct, the fractional factorial design of resolution R will project into a full factorial in the $R - 1$ significant factors. This process is illustrated in Figure 8-2 for the 2^{3-1}_{III} design, which projects into a 2^2 design in every subset of two factors.

Because the maximum possible resolution of a one-half fraction of the 2^k design is $R = k$, every 2^{k-1} design will project into a full factorial in any $(k - 1)$ of the original k factors. Furthermore, a 2^{k-1} design may be projected into two replicates of a full factorial in any subset of $k - 2$ factors, four replicates of a full factorial in any subset of $k - 3$ factors, and so on.

EXAMPLE 8-1

Consider the filtration rate experiment in Example 6-2. The original design, shown in Table 6-10, is a single replicate of the 2^4 design. In that example, we found that the main effects A, C, and D and the interactions AC and AD were different from zero. We will now return to this experiment and simulate what would have happened if a half-fraction of the 2^4 design had been run instead of the full factorial.

We will use the 2^{4-1} design with $I = ABCD$, because this choice of generator will result in a design of the highest possible resolution (IV). To construct the design, we first write down the basic design, which is a 2^3 design, as shown in the first three columns of Table 8-3. This basic design has the necessary number of runs (eight) but only three columns (factors). To find the fourth factor levels, solve $I = ABCD$ for D, or $D = ABC$. Thus, the level of D in each run is the product of the plus and minus signs in columns

Table 8-3 The 2^{4-1}_{IV} Design with the Defining Relation $I = ABCD$

	Basic Design					
Run	A	B	C	$D = ABC$	Treatment Combination	Filtration Rate
1	−	−	−	−	(1)	45
2	+	−	−	+	ad	100
3	−	+	−	+	bd	45
4	+	+	−	−	ab	65
5	−	−	+	+	cd	75
6	+	−	+	−	ac	60
7	−	+	+	−	bc	80
8	+	+	+	+	$abcd$	96

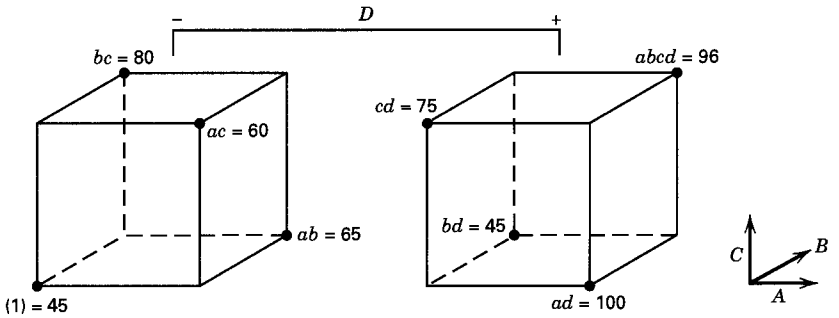


Figure 8-3 The 2_{IV}^{4-1} design for the filtration rate experiment of Example 8-1.

A, B, and C. The process is illustrated in Table 8-3. Because the generator $ABCD$ is positive, this 2_{IV}^{4-1} design is the principal fraction. The design is shown graphically in Figure 8-3.

Using the defining relation, we note that each main effect is aliased with a three-factor interaction; that is, $A = A^2BCD = BCD$, $B = AB^2CD = ACD$, $C = ABC^2D = ABD$, and $D = ABCD^2 = ABC$. Furthermore, every two-factor interaction is aliased with another two-factor interaction. These alias relationships are $AB = CD$, $AC = BD$, and $BC = AD$. The four main effects plus the three two-factor interaction alias pairs account for the seven degrees of freedom for the design.

At this point, we would normally randomize the eight runs and perform the experiment. Because we have already run the full 2^4 design, we will simply select the eight observed filtration rates from Example 6-2 that correspond to the runs in the 2_{IV}^{4-1} design. These observations are shown in the last column of Table 8-3 and are also shown in Figure 8-3.

The estimates of the effects obtained from this 2_{IV}^{4-1} design are shown in Table 8-4. To illustrate the calculations, the linear combination of observations associated with the A effect is

$$\ell_A = \tfrac{1}{4}(-45 + 100 - 45 + 65 - 75 + 60 - 80 + 96) = 19.00 \rightarrow A + BCD$$

whereas for the AB effect, we would obtain

$$\ell_{AB} = \tfrac{1}{4}(45 - 100 - 45 + 65 + 75 - 60 - 80 + 96) = -1.00 \rightarrow AB + CD$$

From inspection of the information in Table 8-4, it is not unreasonable to conclude that the main effects A, C, and D are large. Furthermore, if A, C, and D are the important main effects, then it is logical to conclude that the two interaction alias chains $AC + BD$

Table 8-4 Estimates of Effects and Aliases from Example 8-1[a]

Estimate		Alias Structure
$\ell_A =$	19.00	$\ell_A \rightarrow \boldsymbol{A} + BCD$
$\ell_B =$	1.50	$\ell_B \rightarrow \boldsymbol{B} + ACD$
$\ell_C =$	14.00	$\ell_C \rightarrow \boldsymbol{C} + ABD$
$\ell_D =$	16.50	$\ell_D \rightarrow \boldsymbol{D} + ABC$
$\ell_{AB} =$	−1.00	$\ell_{AB} \rightarrow AB + CD$
$\ell_{AC} =$	−18.50	$\ell_{AC} \rightarrow \boldsymbol{AC} + BD$
$\ell_{AD} =$	19.00	$\ell_{AD} \rightarrow \boldsymbol{AD} + BC$

[a] Significant effects are shown in boldface type.

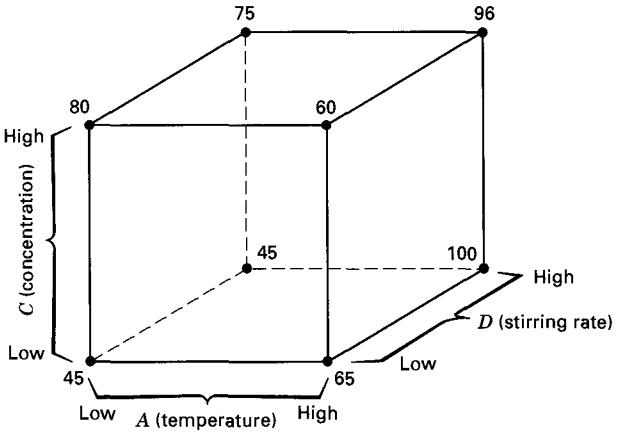


Figure 8-4 Projection of the 2^{4-1}_{IV} design into a 2^3 design in A, C, and D for Example 8-1.

and $AD + BC$ have large effects because the AC and AD interactions are also significant. In other words, if A, C, and D are significant then the significant interactions are most likely AC and AD. This is an application of **Ockham's razor** (after William of Ockham), a scientific principle that when one is confronted with several different possible interpretations of a phenomena, the simplest interpretation is usually the correct one. Note that this interpretation agrees with the conclusions from the analysis of the complete 2^4 design in Example 6-2.

Because factor B is not significant, we may drop it from consideration. Consequently, we may project this 2^{4-1}_{IV} design into a single replicate of the 2^3 design in factors A, C, and D, as shown in Figure 8-4. Visual examination of this cube plot makes us more comfortable with the conclusions reached above. Notice that if the temperature (A) is at the low level, the concentration (C) has a large positive effect, whereas if the temperature is at the high level, the concentration has a very small effect. This is probably due to an AC interaction. Furthermore, if the temperature is at the low level, the effect of the stirring rate (D) is negligible, whereas if the temperature is at the high level, the stirring rate has a large positive effect. This is probably due to the AD interaction tentatively identified previously.

Based on the above analysis, we can now obtain a model to predict filtration rate over the experimental region. This model is

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_3 x_3 + \hat{\beta}_4 x_4 + \hat{\beta}_{13} x_1 x_3 + \hat{\beta}_{14} x_1 x_4$$

where x_1, x_3, and x_4 are coded variables ($-1 \leq x_i \leq +1$) that represent A, C, and D, and the $\hat{\beta}$'s are regression coefficients that can be obtained from the effect estimates as we did previously. Therefore, the prediction equation is

$$\hat{y} = 70.75 + \left(\frac{19.00}{2}\right) x_1 + \left(\frac{14.00}{2}\right) x_3 + \left(\frac{16.50}{2}\right) x_4 + \left(\frac{-18.50}{2}\right) x_1 x_3 + \left(\frac{19.00}{2}\right) x$$

Remember that the intercept $\hat{\beta}_0$ is the average of all responses at the eight runs in the design. This model is very similar to the one that resulted from the full 2^k factorial design in Example 6-2.

EXAMPLE 8-2

A 2^{5-1} Design Used for Process Improvement

Five factors in a manufacturing process for an integrated circuit were investigated in a 2^{5-1} design with the objective of improving the process yield. The five factors were A = aperture setting (small, large), B = exposure time (20 percent below nominal, 20 percent above nominal), C = develop time (30 s, 45 s), D = mask dimension (small, large), and E = etch time (14.5 min, 15.5 min). The construction of the 2^{5-1} design is shown in Table 8-5. Notice that the design was constructed by writing down the basic design having 16 runs (a 2^4 design in A, B, C, and D), selecting $ABCDE$ as the generator, and then setting the levels of the fifth factor $E = ABCD$. Figure 8-5 (on page 312) gives a pictorial representation of the design.

The defining relation for the design is $I = ABCDE$. Consequently, every main effect is aliased with a four-factor interaction (for example, $\ell_A \rightarrow A + BCDE$), and every two-factor interaction is aliased with a three-factor interaction (for example, $\ell_{AB} \rightarrow AB + CDE$). Thus, the design is of resolution V. We would expect this 2^{5-1} design to provide excellent information concerning the main effects and two-factor interactions.

Table 8-6 (on page 312) contains the effect estimates, sums of squares, and model regression coefficients for the 15 effects from this experiment. Figure 8-6 (on page 313) presents a normal probability plot of the effect estimates from this experiment. The main effects of A, B, and C and the AB interaction are large. Remember that, because of aliasing, these effects are really $A + BCDE$, $B + ACDE$, $C + ABDE$, and $AB + CDE$. However, because it seems plausible that three-factor and higher interactions are negligible, we feel safe in concluding that only A, B ,C, and AB are important effects.

Table 8-7 (page 313) summarizes the analysis of variance for this experiment. The model sum of squares is $SS_{\text{Model}} = SS_A + SS_B + SS_C + SS_{AB} = 5747.25$, and this accounts for over 99 percent of the total variability in yield. Figure 8-7 (paged 313) presents a

Table 8-5 A 2^{5-1} Design for Example 8-2

	Basic Design						
Run	A	B	C	D	$E = ABCD$	Treatment Combination	Yield
1	−	−	−	−	+	*e*	8
2	+	−	−	−	−	*a*	9
3	−	+	−	−	−	*b*	34
4	+	+	−	−	+	*abe*	52
5	−	−	+	−	−	*c*	16
6	+	−	+	−	+	*ace*	22
7	−	+	+	−	+	*bce*	45
8	+	+	+	−	−	*abc*	60
9	−	−	−	+	−	*d*	6
10	+	−	−	+	+	*ade*	10
11	−	+	−	+	+	*bde*	30
12	+	+	−	+	−	*abd*	50
13	−	−	+	+	+	*cde*	15
14	+	−	+	+	−	*acd*	21
15	−	+	+	+	−	*bcd*	44
16	+	+	+	+	+	*abcde*	63

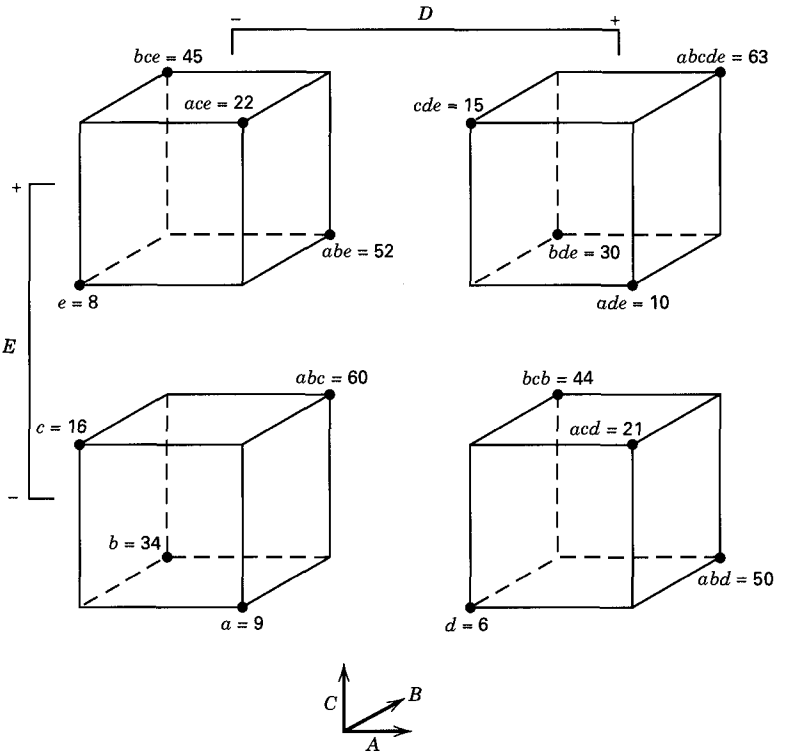


Figure 8-5 The 2_V^{5-1} design for Example 8-2.

Table 8-6 Effects, Regression Coefficients, and Sums of Squares for Example 8-2

Variable	Name	−1 Level	+1 Level
A	Aperture	−1.000	1.000
B	Develop time	−1.000	1.000
C	Exposure time	−1.000	1.000
D	Mask dimension	−1.000	1.000
E	Etch time	−1.000	1.000

Variable	Regression Coefficient	Estimated Effect	Sum of Squares
Overall Average	30.3125		
A	5.5625	11.1250	495.062
B	16.9375	33.8750	4590.062
C	5.4375	10.8750	473.062
D	−0.4375	−0.8750	3.063
E	0.3125	0.6250	1.563
AB	3.4375	6.8750	189.063
AC	0.1875	0.3750	0.563
AD	0.5625	1.1250	5.063
AE	0.5625	1.1250	5.063
BC	0.3125	0.6250	1.563
BD	−0.0625	−0.1250	0.063
BE	−0.0625	−0.1250	0.063
CD	0.4375	0.8750	3.063
CE	0.1875	0.3750	0.563
DE	−0.6875	−1.3750	7.563

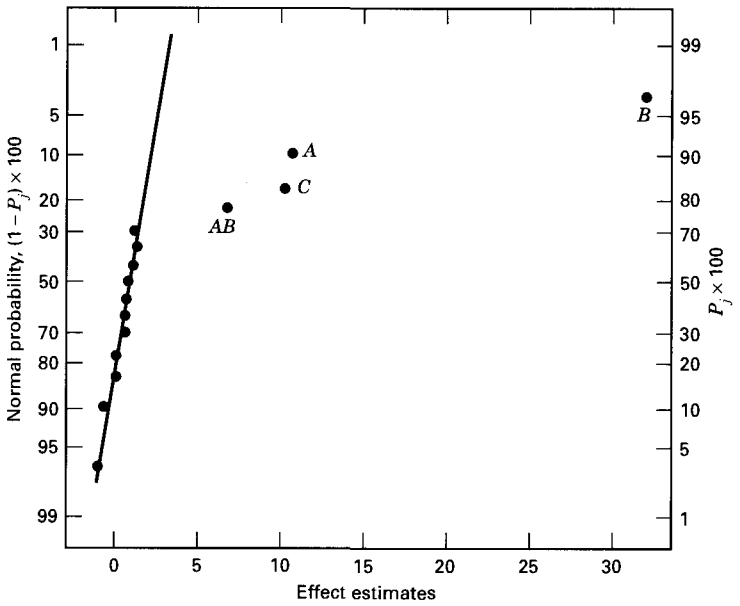


Figure 8-6 Normal probability plot of effects for Example 8-2.

Table 8-7 Analysis of Variance for Example 8-2

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
A (Aperture)	495.0625	1	495.0625	193.20	<0.0001
B (Exposure time)	4590.0625	1	4590.0625	1791.24	<0.0001
C (Develop time)	473.0625	1	473.0625	184.61	<0.0001
AB	189.0625	1	189.0625	73.78	<0.0001
Error	28.1875	11	2.5625		
Total	5775.4375	15			

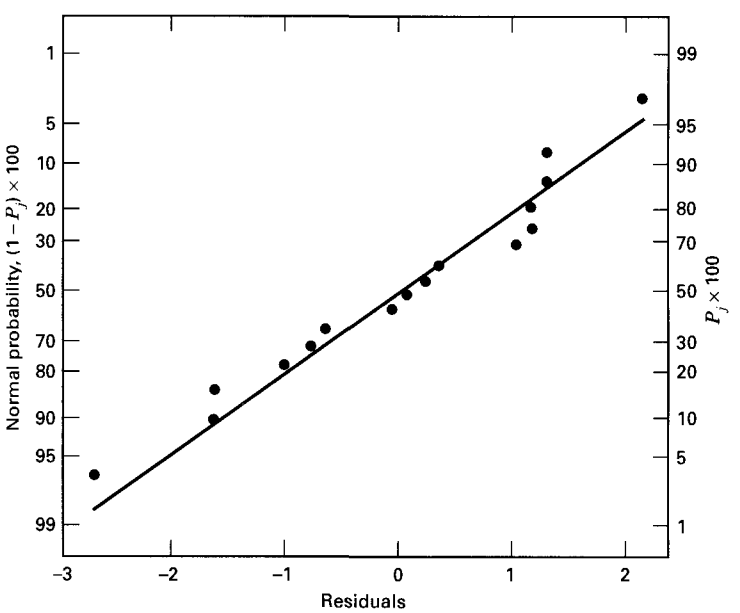


Figure 8-7 Normal probability plot of the residuals for Example 8-2.

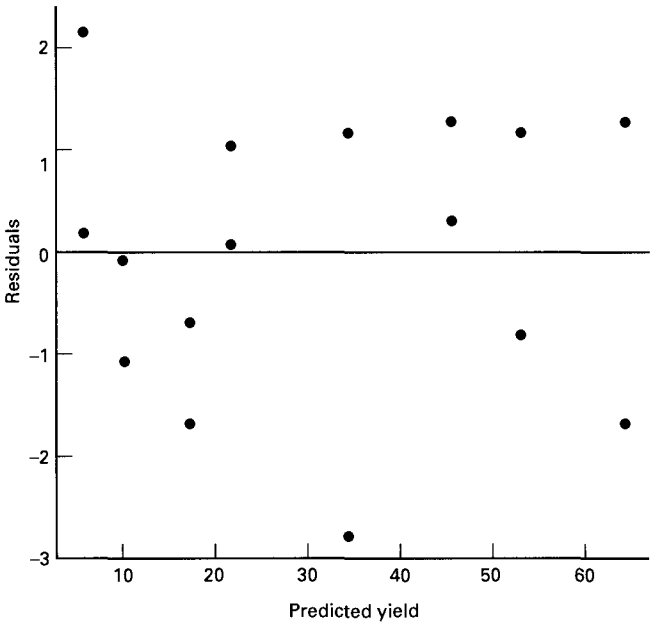


Figure 8-8 Plot of residuals versus predicted yield for Example 8-2.

normal probability plot of the residuals, and Figure 8-8 is a plot of the residuals versus the predicted values. Both plots are satisfactory.

The three factors A, B, and C have large positive effects. The AB or aperture exposure time interaction is plotted in Figure 8-9. This plot confirms that the yields are higher when both A and B are at the high level.

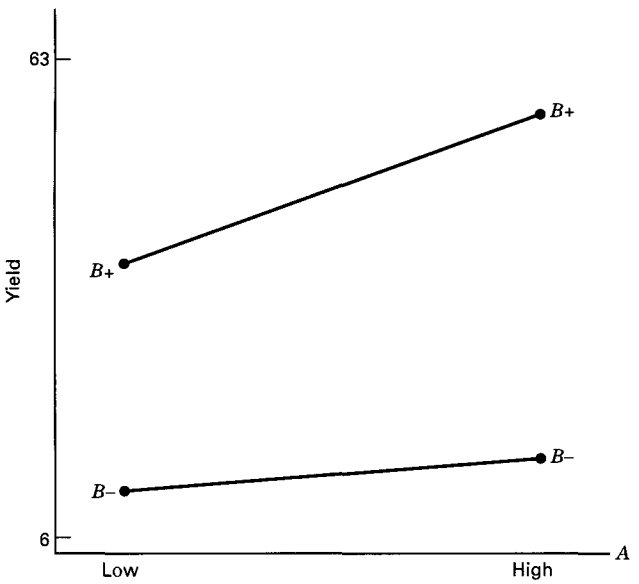


Figure 8-9 Aperture–exposure time interaction for Example 8-2.

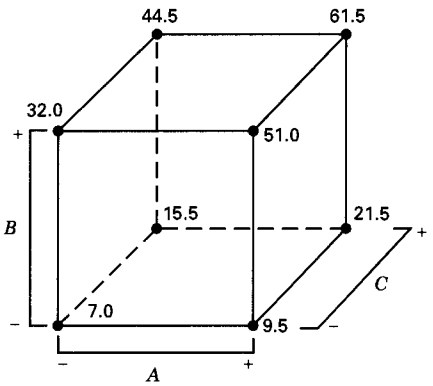


Figure 8-10 Projection of the 2_V^{5-1} design in Example 8-2 into two replicates of a 2^3 design in the factors A, B, and C.

The 2^{5-1} design will collapse into two replicates of a 2^3 design in any three of the original five factors. (Looking at Figure 8-5 will help you visualize this.) Figure 8-10 is a cube plot in the factors A, B, and C with the average yields superimposed on the eight corners. It is clear from inspection of the cube plot that highest yields are achieved with A, B, and C all at the high level. Factors D and E have little effect on average process yield and may be set to values that optimize other objectives (such as cost).

Sequences of Fractional Factorials

Using fractional factorial designs often leads to great economy and efficiency in experimentation, particularly if the runs can be made **sequentially**. For example, suppose that we are investigating $k = 4$ factors ($2^4 = 16$ runs). It is almost always preferable to run a 2_{IV}^{4-1} fractional design (eight runs), analyze the results, and then decide on the best set of runs to perform next. If it is necessary to resolve ambiguities, we can always run the alternate fraction and complete the 2^4 design. When this method is used to complete the design, both one-half fractions represent **blocks** of the complete design with the highest-order interaction confounded with blocks (here $ABCD$ would be confounded). Thus, sequential experimentation has the result of losing information only on the highest-order interaction. Its advantage is that in many cases we learn enough from the one-half fraction to proceed to the next stage of experimentation, which might involve adding or removing factors, changing responses, or varying some of the factors over new ranges. Some of these possibilities are illustrated graphically in Figure 8-11 on the following page.

EXAMPLE 8-3

Reconsider the experiment in Example 8-2. We have used a 2_{IV}^{4-1} design and tentatively identified three large main effects—A, C, and D. There are two large effects associated with two-factor interactions, $AC + BD$ and $AD + BC$. In Example 8-2, we used the fact that the main effect of B was negligible to tentatively conclude that the important inter-

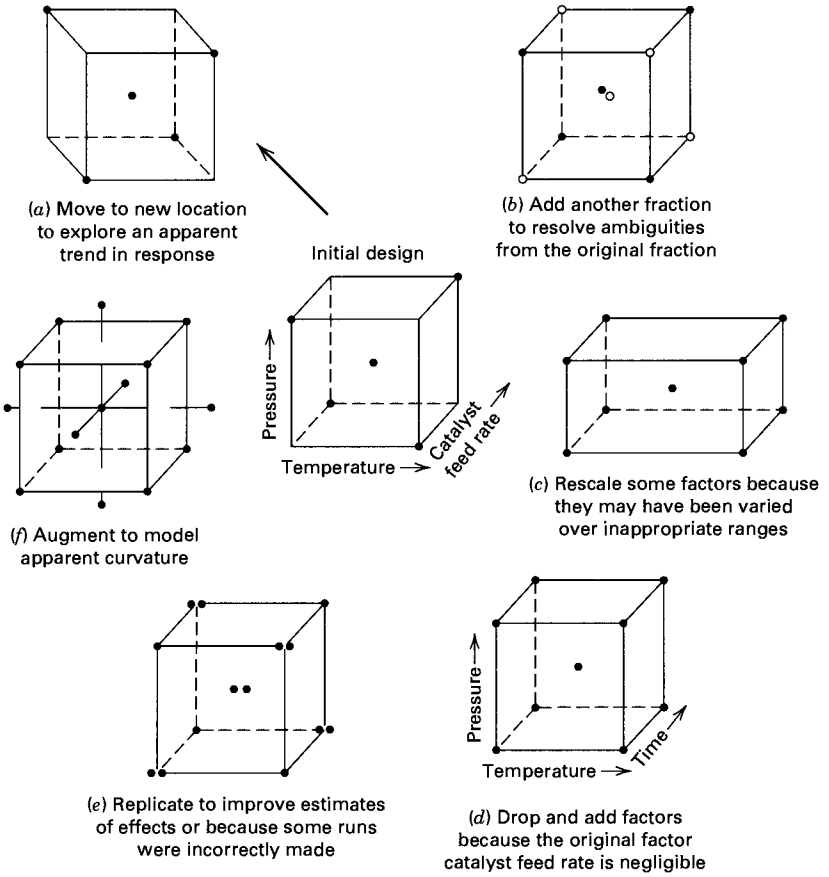

(a) Move to new location to explore an apparent trend in response
Initial design
(b) Add another fraction to resolve ambiguities from the original fraction
Pressure
Temperature
Catalyst feed rate
(c) Rescale some factors because they may have been varied over inappropriate ranges
(f) Augment to model apparent curvature
(e) Replicate to improve estimates of effects or because some runs were incorrectly made
Pressure
Temperature
Time
(d) Drop and add factors because the original factor catalyst feed rate is negligible

Figure 8-11 Possibilities for follow-up experimentation after a fractional factorial experiment (adapted from Box (1992–1993), with permission of the publisher).

actions were AC and AD. Sometimes the experimenter will have process knowledge that can assist in discriminating between interactions likely to be important. However, we can always isolate the significant interaction by running the alternate fraction, given by $I = -ABCD$. It is straightforward to show that the design and the responses are as follows:

	Basic Design					
Run	A	B	C	$D = -ABC$	Treatment Combination	Filtration Rate
1	−	−	−	+	d	43
2	+	−	−	−	a	71
3	−	+	−	−	b	48
4	+	+	−	+	abd	104
5	−	−	+	−	c	68
6	+	−	+	+	acd	86
7	−	+	+	+	bcd	70
8	+	+	+	−	abc	65

The linear combinations of observations obtained from this alternate fraction are

$$\begin{aligned}
\ell'_A &= 24.25 \rightarrow A - BCD \\
\ell'_B &= 4.75 \rightarrow B - ACD \\
\ell'_C &= 5.75 \rightarrow C - ABD \\
\ell'_D &= 12.75 \rightarrow D - ABC \\
\ell'_{AB} &= 1.25 \rightarrow AB - CD \\
\ell'_{AC} &= -17.75 \rightarrow AC - BD \\
\ell'_{AD} &= 14.25 \rightarrow AD - BC
\end{aligned}$$

These estimates may be combined with those obtained from the original one-half fraction to yield the following estimates of the effects:

i	From $\frac{1}{2}(\ell_i + \ell'_i)$	From $\frac{1}{2}(\ell_i - \ell'_i)$
A	$21.63 \rightarrow A$	$-2.63 \rightarrow BCD$
B	$3.13 \rightarrow B$	$-1.63 \rightarrow ACD$
C	$9.88 \rightarrow C$	$4.13 \rightarrow ABD$
D	$14.63 \rightarrow D$	$1.88 \rightarrow ABC$
AB	$0.13 \rightarrow AB$	$-1.13 \rightarrow CD$
AC	$-18.13 \rightarrow AC$	$-0.38 \rightarrow BD$
AD	$16.63 \rightarrow AD$	$2.38 \rightarrow BC$

These estimates agree exactly with those from the original analysis of the data as a single replicate of a 2^4 factorial design, as reported in Example 6-2. Clearly, it is the AC and AD interactions that are large.

Adding the alternate fraction to the principal fraction may be thought of as a type of **confirmation experiment** in that it provides information that will allow us to strengthen our initial conclusions about the two-factor interaction effects. We will investigate some other aspects of combining fractional factorials to isolate interactions in Section 8-5. Sometimes a confirmation experiment is not this elaborate. For example, one could use the model equation to predict the response at a point of interest within the design space (not one of the points in the current design), then actually run that trial (perhaps several times) and use the comparison between predicted and observed response to confirm the results.

8-3 THE ONE-QUARTER FRACTION OF THE 2^k DESIGN

For a moderately large number of factors, smaller fractions of the 2^k design are frequently useful. Consider a one-quarter fraction of the 2^k design. This design contains 2^{k-2} runs and is usually called a $\mathbf{2^{k-2}}$ **fractional factorial**.

The 2^{k-2} design may be constructed by first writing down a **basic design** consisting of the runs associated with a full factorial in $k - 2$ factors and then associating the two additional columns with appropriately chosen interactions involving the first $k - 2$ factors. Thus, a one-quarter fraction of the 2^k design has two generators. If P and Q represent

the generators chosen, then $I = P$ and $I = Q$ are called the **generating relations** for the design. The signs of P and Q (either + or −) determine which one of the one-quarter fractions is produced. All four fractions associated with the choice of **generators** $\pm P$ and $\pm Q$ are members of the same **family**. The fraction for which both P and Q are positive is the principal fraction.

The **complete defining relation** for the design consists of all the columns that are equal to the identity column I. These will consist of P, Q, and their **generalized interaction** PQ; that is, the defining relation is $I = P = Q = PQ$. We call the elements P, Q, and PQ in the defining relation **words**. The aliases of any effect are produced by the multiplication of the column for that effect by each word in the defining relation. Clearly, each effect has *three* aliases. The experimenter should be careful in choosing the generators so that potentially important effects are not aliased with each other.

As an example, consider the 2^{6-2} design. Suppose we choose $I = ABCE$ and $I = BCDF$ as the design generators. Now the generalized interaction of the generators $ABCE$ and $BCDF$ is $ADEF$; therefore, the complete defining relation for this design is

$$I = ABCE = BCDF = ADEF$$

Consequently, this is a resolution IV design. To find the aliases of any effect (e.g., A), multiply that effect by each word in the defining relation. For A, this produces

$$A = BCE = ABCDF = DEF$$

It is easy to verify that every main effect is aliased by three- and five-factor interactions, whereas two-factor interactions are aliased with each other and with higher-order interactions. Thus, when we estimate A, for example, we are really estimating $A + BCE + DEF + ABCDF$. The complete alias structure of this design is shown in Table 8-8. If three-factor and higher interactions are negligible, this design gives clear estimates of the main effects.

To construct the design, first write down the **basic design**, which consists of the 16 runs for a full $2^{6-2} = 2^4$ design in A, B, C, and D. Then the two factors E and F are added by associating their plus and minus levels with the plus and minus signs of the interactions ABC and BCD, respectively. This procedure is shown in Table 8-9.

Another way to construct this design is to derive the four blocks of the 2^6 design with $ABCE$ and $BCDF$ confounded and then choose the block with treatment combinations that are positive on $ABCE$ and $BCDF$. This would be a 2^{6-2} fractional factorial with generating relations $I = ABCE$ and $I = BCDF$, and because both generators $ABCE$ and $BCDF$ are positive, this is the principal fraction.

There are, of course, three **alternate fractions** of this particular 2^{6-2}_{IV} design. They

Table 8-8 Alias Structure for the 2^{6-2}_{IV} Design with I = ABCE = BCDF = ADEF

$A = BCE = DEF = ABCDF$	$AB = CE = ACDF = BDEF$
$B = ACE = CDF = ABDEF$	$AC = BE = ABDF = CDEF$
$C = ABE = BDF = ACDEF$	$AD = EF = BCDE = ABCF$
$D = BCF = AEF = ABCDE$	$AE = BC = DF = ABCDEF$
$E = ABC = ADF = BCDEF$	$AF = DE = BCEF = ABCD$
$F = BCD = ADE = ABCEF$	$BD = CF = ACDE = ABEF$
	$BF = CD = ACEF = ABDE$
$ABD = CDE = ACF = BEF$	
$ACD = BDE = ABF = CEF$	

Table 8-9 Construction of the 2_{IV}^{6-2} Design with the Generators $I = ABCE$ and $I = BCDF$

	Basic Design					
Run	A	B	C	D	$E = ABC$	$F = BCD$
1	−	−	−	−	−	−
2	+	−	−	−	+	−
3	−	+	−	−	+	+
4	+	+	−	−	−	+
5	−	−	+	−	+	+
6	+	−	+	−	−	+
7	−	+	+	−	−	−
8	+	+	+	−	+	−
9	−	−	−	+	−	+
10	+	−	−	+	+	+
11	−	+	−	+	+	−
12	+	+	−	+	−	−
13	−	−	+	+	+	−
14	+	−	+	+	−	−
15	−	+	+	+	−	+
16	+	+	+	+	+	+

are the fractions with generating relationships $I = ABCE$ and $I = -BCDF$; $I = -ABCE$ and $I = BCDF$; and $I = -ABCE$ and $I = -BCDF$. These fractions may be easily constructed by the method shown in Table 8-9. For example, if we wish to find the fraction for which $I = ABCE$ and $I = -BCDF$, then in the last column of Table 8-9 we set $F = -BCD$, and the column of levels for factor F becomes

$$++---++--+++--$$

The complete defining relation for this alternate fraction is $I = ABCE = -BCDF = -ADEF$. Certain signs in the alias structure in Table 8-9 are now changed; for instance, the aliases of A are $A = BCE = -DEF = -ABCDF$. Thus, the linear combination of the observations ℓ_A actually estimates $A + BCE - DEF - ABCDF$.

Finally, note that the 2_{IV}^{6-2} fractional factorial will project into a single replicate of a 2^4 design in any subset of four factors that is not a word in the defining relation. It also collapses to a replicated one-half fraction of a 2^4 in any subset of four factors that is a word in the defining relation. Thus, the design in Table 8-9 becomes two replicates of a 2^{4-1} in the factors $ABCE$, $BCDF$, and $ADEF$, because these are the words in the defining relation. There are 12 other combinations of the six factors, such as $ABCD$, $ABCF$, and so on, for which the design projects to a single replicate of the 2^4. This design also collapses to two replicates of a 2^3 in *any* subset of three of the six factors or four replicates of a 2^2 in any subset of two factors.

In general, any 2^{k-2} fractional factorial design can be collapsed into either a full factorial or a fractional factorial in some subset of $r \leq k - 2$ of the original factors. Those subsets of variables that form full factorials are not words in the complete defining relation.

EXAMPLE 8-4

Parts manufactured in an injection molding process are showing excessive shrinkage. This is causing problems in assembly operations downstream from the injection molding area. A quality improvement team has decided to use a designed experiment to study the

injection molding process so that shrinkage can be reduced. The team decides to investigate six factors—mold temperature (A), screw speed (B), holding time (C), cycle time (D), gate size (E), and holding pressure (F)—each at two levels, with the objective of learning how each factor affects shrinkage and also, something about how the factors interact.

The team decides to use the 16-run two-level fractional factorial design in Table 8-9. The design is shown again in Table 8-10, along with the observed shrinkage ($\times$ 10) for the test part produced at each of the 16 runs in the design. Table 8-11 (on the next page) shows the effect estimates, sums of squares, and the regression coefficients for this experiment.

A normal probability plot of the effect estimates from this experiment is shown in Figure 8-12 (on the facing page). The only large effects are A (mold temperature), B (screw speed), and the AB interaction. In light of the alias relationships in Table 8-8, it seems reasonable to adopt these conclusions tentatively. The plot of the AB interaction in Figure 8-13 (on page 322) shows that the process is very insensitive to temperature if the screw speed is at the low level but very sensitive to temperature if the screw speed is at the high level. With the screw speed at the low level, the process should produce an average shrinkage of around 10 percent regardless of the temperature level chosen.

Based on this initial analysis, the team decides to set both the mold temperature and the screw speed at the low level. This set of conditions will reduce the *mean* shrinkage of parts to around 10 percent. However, the variability in shrinkage from part to part is still a potential problem. In effect, the mean shrinkage can be adequately reduced by the above modifications; however, the part-to-part variability in shrinkage over a production run could still cause problems in assembly. One way to address this issue is to see if any of the process factors affect the *variability* in parts shrinkage.

Figure 8-14 (on page 322) presents the normal probability plot of the residuals. This plot appears satisfactory. The plots of residuals versus each factor were then constructed.

Table 8-10 A 2_{IV}^{6-2} Design for the Injection Molding Experiment in Example 8-4

	Basic Design						Observed Shrinkage
Run	A	B	C	D	$E = ABC$	$F = BCD$	($\times$ 10)
1	−	−	−	−	−	−	6
2	+	−	−	−	+	−	10
3	−	+	−	−	+	+	32
4	+	+	−	−	−	+	60
5	−	−	+	−	+	+	4
6	+	−	+	−	−	+	15
7	−	+	+	−	−	−	26
8	+	+	+	−	+	−	60
9	−	−	−	+	−	+	8
10	+	−	−	+	+	+	12
11	−	+	−	+	+	−	34
12	+	+	−	+	−	−	60
13	−	−	+	+	+	−	16
14	+	−	+	+	−	−	5
15	−	+	+	+	−	+	37
16	+	+	+	+	+	+	52

Table 8-11 Effects, Sums of Squares, and Regression Coefficients for Example 8-4

Variable	Name	−1 Level	+1 Level
A	mold_temp	−1.000	1.000
B	screw_spd	−1.000	1.000
C	hold_time	−1.000	1.000
D	cycle_time	−1.000	1.000
E	gate_size	−1.000	1.000
F	hold_press	−1.000	1.000

Variable[a]	Regression Coefficient	Estimated Effect	Sum of Squares
Overall Average	27.3125		
A	6.9375	13.8750	770.062
B	17.8125	35.6250	5076.562
C	−0.4375	−0.8750	3.063
D	0.6875	1.3750	7.563
E	0.1875	0.3750	0.563
F	0.1875	0.3750	0.563
AB + *CE*	5.9375	11.8750	564.063
AC + *BE*	−0.8125	−1.6250	10.562
AD + *EF*	−2.6875	−5.3750	115.562
AE + *BC* + *DF*	−0.9375	−1.8750	14.063
AF + *DE*	0.3125	0.6250	1.563
BD + *CF*	−0.0625	−0.1250	0.063
BF + *CD*	−0.0625	−0.1250	0.063
ABD	0.0625	0.1250	0.063
ABF	−2.4375	−4.8750	95.063

[a] Only main effects and two-factor interactions.

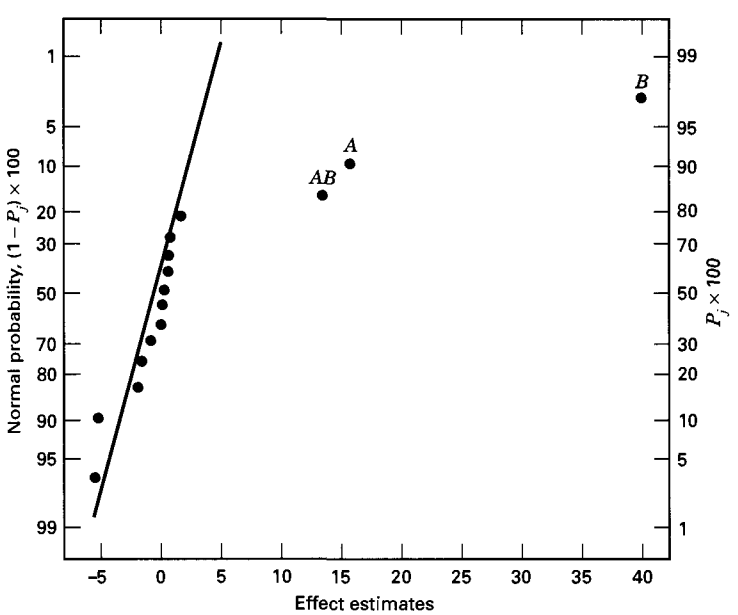


Figure 8-12 Normal probability plot of effects for Example 8-4.

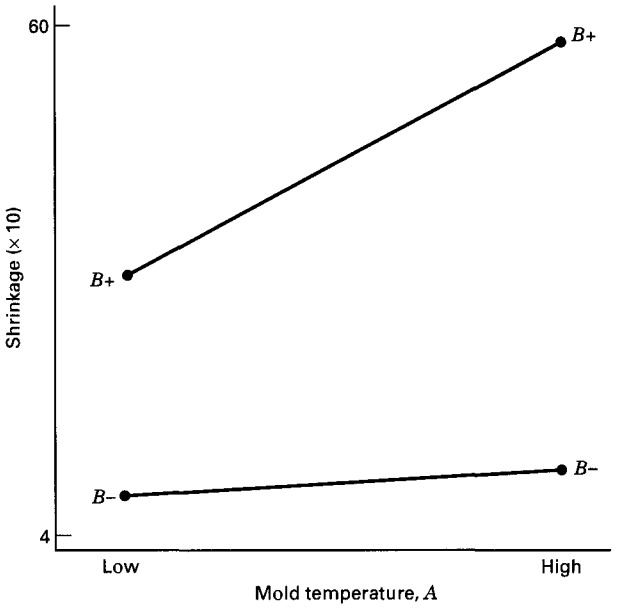


Figure 8-13 Plot of *AB* (mold temperature–screw speed) interaction for Example 8-4.

One of these plots, that for residuals versus factor C (holding time), is shown in Figure 8-15. The plot reveals that there is much less scatter in the residuals at the low holding time than at the high holding time. These residuals were obtained in the usual way from a model for predicted shrinkage:

$$\begin{aligned}\hat{y} &= \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_{12} x_1 x_2 \\ &= 27.3125 + 6.9375 x_1 + 17.8125 x_2 + 5.9375 x_1 x_2\end{aligned}$$

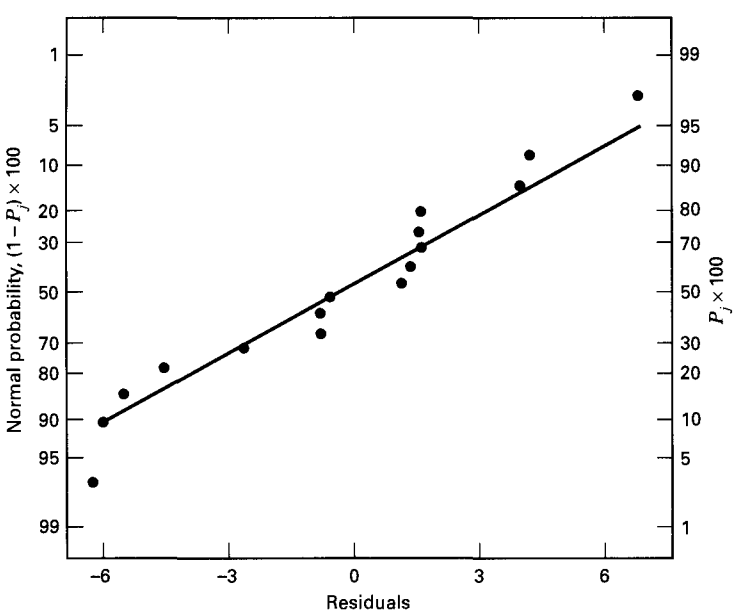


Figure 8-14 Normal probability plot of residuals for Example 8-4.

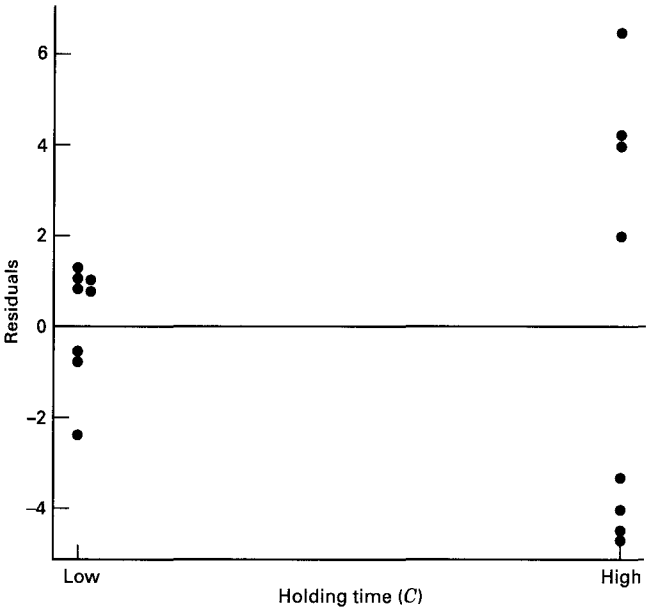


Figure 8-15 Residuals versus holding time (C) for Example 8-4.

where x_1, x_2, and x_1x_2 are coded variables that correspond to the factors A and B and the AB interaction. The residuals are then

$$e = y - \hat{y}$$

The regression model used to produce the residuals essentially removes the **location effects** of A, B, and AB from the data; the residuals therefore contain information about unexplained variability. Figure 8-15 indicates that there is a *pattern* in the variability and that the variability in the shrinkage of parts may be smaller when the holding time is at the low level (please recall that we observed in Chapter 6 that residuals only convey information about dispersion effects when the location or mean model is correct).

This is further amplified by the analysis of residuals shown in Table 8-12 (on page 324). In this table, the residuals are arranged at the low (−) and high (+) levels of each factor, and the standard deviation of the residuals at the low and high levels of each factor have been calculated. Note that the standard deviation of the residuals with C at the low level [$S(C^-) = 1.63$] is considerably smaller than the standard deviation of the residuals with C at the high level [$S(C^+) = 5.70$].

The bottom line of Table 8-12 presents the statistic

$$F_i^* = \ln \frac{S^2(i^+)}{S^2(i^-)}$$

Recall that if the variances of the residuals at the high (+) and low (−) levels of factor i are equal, then this ratio is approximately normally distributed with mean zero, and it can be used to judge the difference in the response variability at the two levels of factor i. Because the ratio F_C^* is relatively large, we would conclude that the apparent **dispersion** or **variability effect** observed in Figure 8-15 is real. Thus, setting the holding time at its low level would contribute to reducing the variability in shrinkage from part to part

Table 8-12 Calculation of Dispersion Effects for Example 8-4

Run	A	B	$AB = CE$	C	$AC = BE$	$AE = BC = DF$	E	D	$AD = EF$	$BD = CE$	ABD	$BF = CD$	ACD	F	$AF = DE$	Residual
1	−	−	+	−	+	+	−	−	+	+	−	+	−	−	+	−2.50
2	+	−	−	−	−	+	+	−	−	+	+	+	+	−	−	−0.50
3	−	+	−	−	+	−	+	−	+	−	+	+	−	+	−	−0.25
4	+	+	+	−	−	−	−	−	−	−	−	+	+	+	+	2.00
5	−	−	+	+	−	−	+	−	+	+	−	−	+	+	−	−4.50
6	+	−	−	+	+	−	−	−	−	+	+	−	−	+	+	4.50
7	−	+	−	+	−	+	−	−	+	−	+	−	+	−	+	−6.25
8	+	+	+	+	+	+	+	−	−	−	−	−	−	−	−	2.00
9	−	−	+	−	+	+	−	+	−	−	+	−	+	+	−	−0.50
10	+	−	−	−	−	+	+	+	+	−	−	−	−	+	+	1.50
11	−	+	−	−	+	−	+	+	−	+	−	−	+	−	+	1.75
12	+	+	+	−	−	−	−	+	+	+	+	−	−	−	−	2.00
13	−	−	+	+	−	−	+	+	−	−	+	+	−	−	+	7.50
14	+	−	−	+	+	−	−	+	+	−	−	+	+	−	−	−5.50
15	−	+	−	+	−	+	−	+	−	+	−	+	−	+	−	4.75
16	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	−6.00
$S(i^+)$	3.80	4.01	4.33	5.70	3.68	3.85	4.17	4.64	3.39	4.01	4.72	4.71	3.50	3.88	4.87	
$S(i^-)$	4.60	4.41	4.10	1.63	4.53	4.33	4.25	3.59	2.75	4.41	3.51	3.65	3.12	4.52	3.40	
F_i^*	−0.38	−0.19	0.11	2.50	−0.42	−0.23	−0.04	0.51	0.42	−0.19	0.59	0.51	0.23	−0.31	0.72	

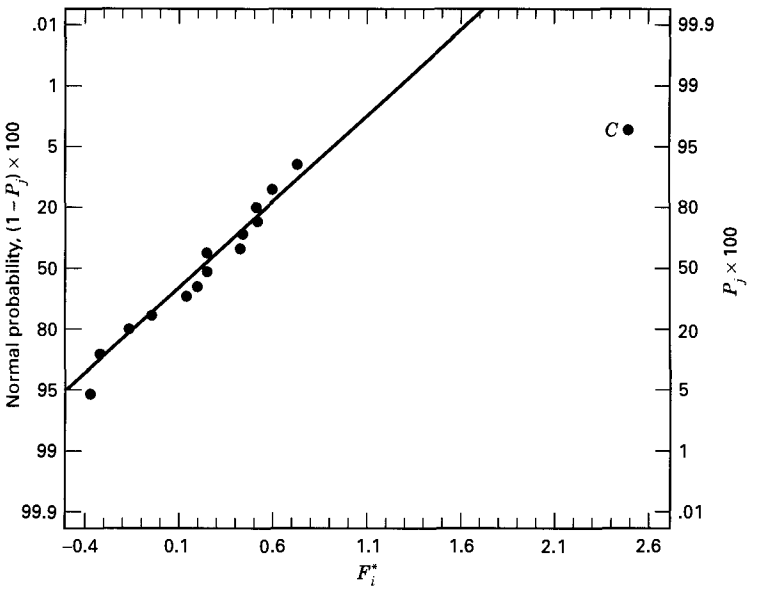


Figure 8-16 Normal probability plot of the dispersion effects F_i^* for Example 8-4.

during a production run. Figure 8-16 presents a normal probability plot of the F_i^* values in Table 8-12; this also indicates that factor C has a large dispersion effect.

Figure 8-17 shows the data from this experiment projected onto a cube in the factors A, B, and C. The average observed shrinkage and the range of observed shrinkage are shown at each corner of the cube. From inspection of this figure, we see that running the process with the screw speed (B) at the low level is the key to reducing average parts shrinkage. If B is low, virtually any combination of temperature (A) and holding time (C) will result in low values of average parts shrinkage. However, from examining the ranges of the shrinkage values at each corner of the cube, it is immediately clear that setting the holding time (C) at the low level is the only reasonable choice if we wish to keep the part-to-part variability in shrinkage low during a production run.

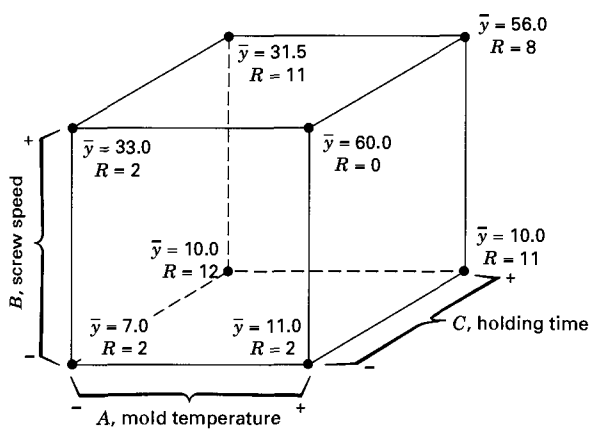


Figure 8-17 Average shrinkage and range of shrinkage in factors A, B, and C for Example 8-4.

8-4 THE GENERAL 2^{k-p} FRACTIONAL FACTORIAL DESIGN

A 2^k fractional factorial design containing 2^{k-p} runs is called a $1/2^p$ fraction of the 2^k design or, more simply, a **2^{k-p} fractional factorial design**. These designs require the selection of p independent generators. The defining relation for the design consists of the p generators initially chosen and their $2^p - p - 1$ generalized interactions. In this section we discuss the construction and analysis of these designs.

The alias structure may be found by multiplying each effect column by the defining relation. Care should be exercised in choosing the generators so that effects of potential interest are not aliased with each other. Each effect has $2^p - 1$ aliases. For moderately large values of k, we usually assume higher-order interactions (say, third- or fourth-order and higher) to be negligible, and this greatly simplifies the alias structure.

It is important to select the p generators for a 2^{k-p} fractional factorial design in such a way that we obtain the best possible alias relationships. A reasonable criterion is to select the generators such that the resulting 2^{k-p} design has the **highest possible resolution**. To illustrate, consider the 2_{IV}^{6-2} design in Table 8-9, where we used the generators $E = ABC$ and $F = BCD$, thereby producing a design of resolution IV. This is the maximum resolution design. If we had selected $E = ABC$ and $F = ABCD$, the complete defining relation would have been $I = ABCE = ABCDF = DEF$, and the design would be of resolution III. Clearly this is an inferior choice because it needlessly sacrifices information about interactions.

Sometimes resolution alone is insufficient to distinguish between designs. For example, consider the three 2_{IV}^{7-2} designs in Table 8-13. All of these designs are of resolution IV, but they have rather different alias structures (we have assumed that three-factor and higher interactions are negligible) with respect to the two-factor interactions. Clearly design A has more aliasing and design C the least, so design C would be the best choice for a 2_{IV}^{7-2}.

The three word lengths in design A are all 4; that is, the word length **pattern** is {4, 4, 4}. For design B it is {4, 4, 6}, and for design C it is {4, 5, 5}. Notice that the defining relation for design C has only one four-letter word, whereas the other designs have two or three. Thus, design C minimizes the number of words in the defining relation that are of minimum length. We call such a design a **minimum aberration design**. Minimizing aberration in a design of resolution R ensures that the design has the minimum number of main effects aliased with interactions of order $R - 1$, the minimum number of two-

Table 8-13 Three Choices of Generators for the 2_{IV}^{7-2} Design

Design A Generators: $F = ABC, G = BCD$ $I = ABCF = BCDG = ADFG$	Design B Generators: $F = ABC, G = ADE$ $I = ABCF = ADEG = BCDEFG$	Design C Generators: $F = ABCD, G = ABDE$ $I = ABCDF = ABDEG = CEFG$
Aliases (Two-Factor Interactions)	Aliases (Two-Factor Interactions)	Aliases (Two-Factor Interactions)
$AB = CF$	$AB = CF$	$CE = FG$
$AC = BF$	$AC = BF$	$CF = EG$
$AD = FG$	$AD = EG$	$CG = EF$
$AG = DF$	$AE = DG$	
$BD = CG$	$AF = BC$	
$BG = CD$	$AG = DE$	
$AF = BC = DG$		

factor interactions aliased with interactions of order $R - 2$, and so forth. Refer to Fries and Hunter (1980) for more details.

Table 8-14 (pages 328–330) presents a selection of 2^{k-p} fractional factorial designs for $k \leq 15$ factors and up to $n \leq 128$ runs. The suggested generators in this table will result in a design of the highest possible resolution. These are also the minimum aberration designs.

The alias relationships for all of the designs in Table 8-14 for which $n \leq 64$ are given in Appendix Table XII(a–w). The alias relationships presented in this table focus on main effects and two- and three-factor interactions. The complete defining relation is given for each design. This appendix table makes it very easy to select a design of sufficient resolution to ensure that any interactions of potential interest can be estimated.

EXAMPLE 8-5

To illustrate the use of Table 8-14, suppose that we have seven factors and that we are interested in estimating the seven main effects and getting some insight regarding the two-factor interactions. We are willing to assume that three-factor and higher interactions are negligible. This information suggests that a resolution IV design would be appropriate.

Table 8-14 shows that there are two resolution IV fractions available: the 2_{IV}^{7-2} with 32 runs and the 2_{IV}^{7-3} with 16 runs. Appendix Table XII contains the complete alias relationships for these two designs. The aliases for the 2_{IV}^{7-3} 16-run design are in Appendix Table XII(i). Notice that all seven main effects are aliased with three-factor interactions. The two-factor interactions are all aliased in groups of three. Therefore, this design will satisfy our objectives; that is, it will allow the estimation of the main effects, and it will give some insight regarding two-factor interactions. It is not necessary to run the 2_{IV}^{7-2} design, which would require 32 runs. Appendix Table XII(j) shows that this design would allow the estimation of all seven main effects and that 15 of the 21 two-factor interactions could also be uniquely estimated. (Recall that three-factor and higher interactions are negligible.) This is more information about interactions than is necessary. The complete design is shown in Table 8-15 (page 330). Notice that it was constructed by starting with the 16-run 2^4 design in A, B, C, and D as the basic design and then adding the three columns $E = ABC$, $F = BCD$, and $G = ACD$. The generators are $I = ABCE$, $I = BCDF$, and $I = ACDG$ (Table 8-14). The complete defining relation is $I = ABCE = BCDF = ADEF = ACDG = BDEG = CEFG = ABFG$.

Analysis of 2^{k-p} Fractional Factorials

There are many computer programs that can be used to analyze the 2^{k-p} fractional factorial design. For example, the Design-Expert program illustrated in Chapter 6 has this capability.

The design may also be analyzed by resorting to first principles; the ith effect is estimated by

$$\ell_i = \frac{2(\text{Contrast}_i)}{N} = \frac{\text{Contrast}_i}{(N/2)}$$

where the Contrast_i is found using the plus and minus signs in column i and $N = 2^{k-p}$ is the total number of observations. The 2^{k-p} design allows only $2^{k-p} - 1$ effects (and their aliases) to be estimated.

Table 8-14 Selected 2^{k-p} Fractional Factorial Designs

Number of Factors, k	Fraction	Number of Runs	Design Generators
3	2_{III}^{3-1}	4	$C = \pm AB$
4	2_{IV}^{4-1}	8	$D = \pm ABC$
5	2_{V}^{5-1}	16	$E = \pm ABCD$
	2_{III}^{5-2}	8	$D = \pm AB$
			$E = \pm AC$
6	2_{VI}^{6-1}	32	$F = \pm ABCDE$
	2_{IV}^{6-2}	16	$E = \pm ABC$
			$F = \pm BCD$
	2_{III}^{6-3}	8	$D = \pm AB$
			$E = \pm AC$
			$F = \pm BC$
7	2_{VII}^{7-1}	64	$G = \pm ABCDEF$
	2_{IV}^{7-2}	32	$F = \pm ABCD$
			$G = \pm ABDE$
	2_{IV}^{7-3}	16	$E = \pm ABC$
			$F = \pm BCD$
			$G = \pm ACD$
	2_{III}^{7-4}	8	$D = \pm AB$
			$E = \pm AC$
			$F = \pm BC$
			$G = \pm ABC$
8	2_{V}^{8-2}	64	$G = \pm ABCD$
			$H = \pm ABEF$
	2_{IV}^{8-3}	32	$F = \pm ABC$
			$G = \pm ABD$
			$H = \pm BCDE$
	2_{IV}^{8-4}	16	$E = \pm BCD$
			$F = \pm ACD$
			$G = \pm ABC$
			$H = \pm ABD$
9	2_{VI}^{9-2}	128	$H = \pm ACDFG$
			$J = \pm BCEFG$
	2_{IV}^{9-3}	64	$G = \pm ABCD$
			$H = \pm ACEF$
			$J = \pm CDEF$
	2_{IV}^{9-4}	32	$F = \pm BCDE$
			$G = \pm ACDE$
			$H = \pm ABDE$
			$J = \pm ABCE$
	2_{III}^{9-5}	16	$E = \pm ABC$
			$F = \pm BCD$
			$G = \pm ACD$
			$H = \pm ABD$
			$J = \pm ABCD$
10	2_{V}^{10-3}	128	$H = \pm ABCG$
			$J = \pm ACDE$
			$K = \pm ACDF$

Table 8-14 (continued)

Number of Factors, k	Fraction	Number of Runs	Design Generators
	2_{IV}^{10-4}	64	$G = \pm BCDF$
			$H = \pm ACDF$
			$J = \pm ABDE$
			$K = \pm ABCE$
	2_{IV}^{10-5}	32	$F = \pm ABCD$
			$G = \pm ABCE$
			$H = \pm ABDE$
			$J = \pm ACDE$
			$K = \pm BCDE$
	2_{III}^{10-6}	16	$E = \pm ABC$
			$F = \pm BCD$
			$G = \pm ACD$
			$H = \pm ABD$
			$J = \pm ABCD$
			$K = \pm AB$
11	2_{IV}^{11-5}	64	$G = \pm CDE$
			$H = \pm ABCD$
			$J = \pm ABF$
			$K = \pm BDEF$
			$L = \pm ADEF$
	2_{IV}^{11-6}	32	$F = \pm ABC$
			$G = \pm BCD$
			$H = \pm CDE$
			$J = \pm ACD$
			$K = \pm ADE$
			$L = \pm BDE$
	2_{III}^{11-7}	16	$E = \pm ABC$
			$F = \pm BCD$
			$G = \pm ACD$
			$H = \pm ABD$
			$J = \pm ABCD$
			$K = \pm AB$
			$L = \pm AC$
12	2_{III}^{12-8}	16	$E = \pm ABC$
			$F = \pm ABD$
			$G = \pm ACD$
			$H = \pm BCD$
			$J = \pm ABCD$
			$K = \pm AB$
			$L = \pm AC$
			$M = \pm AD$
13	2_{III}^{13-9}	16	$E = \pm ABC$
			$F = \pm ABD$
			$G = \pm ACD$
			$H = \pm BCD$
			$J = \pm ABCD$
			$K = \pm AB$

Table 8-14 (continued)

Number of Factors, k	Fraction	Number of Runs	Design Generators
			$L = \pm AC$
			$M = \pm AD$
			$N = \pm BC$
14	2_{III}^{14-10}	16	$E = \pm ABC$
			$F = \pm ABD$
			$G = \pm ACD$
			$H = \pm BCD$
			$J = \pm ABCD$
			$K = \pm AB$
			$L = \pm AC$
			$M = \pm AD$
			$N = \pm BC$
			$O = \pm BD$
15	2_{III}^{15-11}	16	$E = \pm ABC$
			$F = \pm ABD$
			$G = \pm ACD$
			$H = \pm BCD$
			$J = \pm ABCD$
			$K = \pm AB$
			$L = \pm AC$
			$M = \pm AD$
			$N = \pm BC$
			$O = \pm BD$
			$P = \pm CD$

Table 8-15 A 2_{IV}^{7-3} Fractional Factorial Design

	Basic Design						
Run	A	B	C	D	$E = ABC$	$F = BCD$	$G = ACD$
1	−	−	−	−	−	−	−
2	+	−	−	−	+	−	+
3	−	+	−	−	+	+	−
4	+	+	−	−	−	+	+
5	−	−	+	−	+	+	+
6	+	−	+	−	−	+	−
7	−	+	+	−	−	−	+
8	+	+	+	−	+	−	−
9	−	−	−	+	−	+	+
10	+	−	−	+	+	+	−
11	−	+	−	+	+	−	+
12	+	+	−	+	−	−	−
13	−	−	+	+	+	−	−
14	+	−	+	+	−	−	+
15	−	+	+	+	−	+	−
16	+	+	+	+	+	+	+

Projection of the 2^{k-p} Fractional Factorial

The 2^{k-p} design collapses into either a full factorial or a fractional factorial in any subset of $r \leq k - p$ of the original factors. Those subsets of factors providing fractional factorials are subsets appearing as words in the complete defining relation. This is particularly useful in screening experiments when we suspect at the outset of the experiment that most of the original factors will have small effects. The original 2^{k-p} fractional factorial can then be projected into a full factorial, say, in the most interesting factors. Conclusions drawn from designs of this type should be considered tentative and subject to further analysis. It is usually possible to find alternative explanations of the data involving higher-order interactions.

As an example, consider the 2_{IV}^{7-3} design from Example 8-5. This is a 16-run design involving seven factors. It will project into a full factorial in any four of the original seven factors that is not a word in the defining relation. There are 35 subsets of four factors, seven of which appear in the complete defining relation (see Table 8-15). Thus, there are 28 subsets of four factors that would form 2^4 designs. One combination that is obvious upon inspecting Table 8-15 is A, B, C, and D.

To illustrate the usefulness of this projection properly, suppose that we are conducting an experiment to improve the efficiency of a ball mill and the seven factors are as follows:

1. Motor speed
2. Gain
3. Feed mode
4. Feed sizing
5. Material type
6. Screen angle
7. Screen vibration level

We are fairly certain that motor speed, feed mode, feed sizing, and material type will affect efficiency and that these factors may interact. The role of the other three factors is less well-known, but it is likely that they are negligible. A reasonable strategy would be to assign motor speed, feed mode, feed sizing, and material type to columns A, B, C, and D, respectively, in Table 8-15. Gain, screen angle, and screen vibration level would be assigned to columns E, F, and G, respectively. If we are correct and the "minor variables" E, F, and G are negligible, we will be left with a full 2^4 design in the key process variables.

Blocking Fractional Factorials

Occasionally, a fractional factorial design requires so many runs that all of them cannot be made under homogeneous conditions. In these situations, fractional factorials may be confounded in blocks. Appendix Table XII contains recommended blocking arrangements for many of the fractional factorial designs in Table 8-14. The minimum block size for these designs is eight runs.

To illustrate the general procedure, consider the 2_{IV}^{6-2} fractional factorial design with the defining relation $I = ABCE = BCDF = ADEF$ shown in Table 8-10. This fractional design contains 16 treatment combinations. Suppose we wish to run the design in two blocks of eight treatment combinations each. In selecting an interaction to confound with blocks, we note from examining the alias structure in Appendix Table XII(f) that there

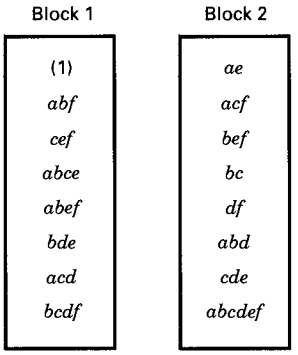


Figure 8-18 The 2_{IV}^{6-2} design in two blocks with ABD confounded.

are two alias sets involving only three-factor interactions. The table suggests selecting ABD (and its aliases) to be confounded with blocks. This would give the two blocks shown in Figure 8-18. Notice that the principal block contains those treatment combinations that have an even number of letters in common with ABD. These are also the treatment combinations for which $L = x_1 + x_2 + x_4 = 0 \pmod 2$.

EXAMPLE 8-6

A five-axis CNC machine is used to machine an impeller used in a jet turbine engine. The blade profiles are an important quality characteristic. Specifically, the deviation of the blade profile from the profile specified on the engineering drawing is of interest. An experiment is run to determine which machine parameters affect profile deviation. The eight factors selected for the design are as follows:

Factor	Low Level (−)	High Level (+)
A = x-Axis shift (0.001 in)	0	15
B = y-Axis shift (0.001 in)	0	15
C = z-Axis shift (0.001 in)	0	15
D = Tool vendor	1	2
E = a-Axis shift (0.001 deg)	0	30
F = Spindle speed (%)	90	110
G = Fixture height (0.001 in)	0	15
H = Feed rate (%)	90	110

One test blade on each part is selected for inspection. The profile deviation is measured using a coordinate measuring machine, and the standard deviation of the difference between the actual profile and the specified profile is used as the response variable.

The machine has four spindles. Because there may be differences in the spindles, the process engineers feel that the spindles should be treated as blocks.

The engineers feel confident that three-factor and higher interactions are not too important, but they are reluctant to ignore the two-factor interactions. From Table 8-14, two designs initially appear appropriate: the 2_{IV}^{8-4} design with 16 runs and the 2_{IV}^{8-3} design

with 32 runs. Appendix Table XII(1) indicates that if the 16-run design is used, there will be fairly extensive aliasing of two-factor interactions. Furthermore, this design cannot be run in four blocks without confounding four two-factor interactions with blocks. Therefore, the experimenters decide to use the 2^{8-3}_{IV} design in four blocks. This confounds one three-factor interaction alias chain and one two-factor interaction (EH) and its three-factor interaction aliases with blocks. The EH interaction is the interaction between the a-axis shift and the feed rate, and the engineers consider an interaction between these two variables to be fairly unlikely.

Table 8-16 contains the design and the resulting responses as standard deviation $\times 10^3$ in. Because the response variable is a standard deviation, it is often best to perform

Table 8-16 The 2^{8-3} Design in Four Blocks for Example 8-6

	Basic Design										
Run	A	B	C	D	E	$F = ABC$	$G = ABD$	$H = BCDE$	Block	Actual Run Order	Standard Deviation ($\times 10^3$ in)
1	−	−	−	−	−	−	−	+	3	18	2.76
2	+	−	−	−	−	+	+	+	2	16	6.18
3	−	+	−	−	−	+	+	−	4	29	2.43
4	+	+	−	−	−	−	−	−	1	4	4.01
5	−	−	+	−	−	+	−	−	1	6	2.48
6	+	−	+	−	−	−	+	−	4	26	5.91
7	−	+	+	−	−	−	+	+	2	14	2.39
8	+	+	+	−	−	+	−	+	3	22	3.35
9	−	−	−	+	−	−	+	−	1	8	4.40
10	+	−	−	+	−	+	−	−	4	32	4.10
11	−	+	−	+	−	+	−	+	2	15	3.22
12	+	+	−	+	−	−	+	+	3	19	3.78
13	−	−	+	+	−	+	+	+	3	24	5.32
14	+	−	+	+	−	−	−	+	2	11	3.87
15	−	+	+	+	−	−	−	−	4	27	3.03
16	+	+	+	+	−	+	+	−	1	3	2.95
17	−	−	−	−	+	−	−	−	2	10	2.64
18	+	−	−	−	+	+	+	−	3	21	5.50
19	−	+	−	−	+	+	+	+	1	7	2.24
20	+	+	−	−	+	−	−	+	4	28	4.28
21	−	−	+	−	+	+	−	+	4	30	2.57
22	+	−	+	−	+	−	+	+	1	2	5.37
23	−	+	+	−	+	−	+	−	3	17	2.11
24	+	+	+	−	+	+	−	−	2	13	4.18
25	−	−	−	+	+	−	+	+	4	25	3.96
26	+	−	−	+	+	+	−	+	1	1	3.27
27	−	+	−	+	+	+	−	−	3	23	3.41
28	+	+	−	+	+	−	+	−	2	12	4.30
29	−	−	+	+	+	+	+	−	2	9	4.44
30	+	−	+	+	+	−	−	−	3	20	3.65
31	−	+	+	+	+	−	−	+	1	5	4.41
32	+	+	+	+	+	+	+	+	4	31	3.40

Table 8-17 Effect Estimates, Regression Coefficients, and Sums of Squares for Example 8-6

Variable	Name	−1 Level	+1 Level
A	*x*-Axis shift	0	15
B	*y*-Axis shift	0	15
C	*z*-Axis shift	0	15
D	Tool vendor	1	2
E	*a*-Axis shift	0	30
F	Spindle speed	90	110
G	Fixture height	0	15
H	Feed rate	90	110

Variable[a]	Regression Coefficient	Estimated Effect	Sum of Squares
Overall Average	1.28007		
A	0.14513	0.29026	0.674020
B	−0.10027	−0.20054	0.321729
C	−0.01288	−0.02576	0.005310
D	0.05407	0.10813	0.093540
E	−2.531E-04	−5.063E-04	2.050E-06
F	−0.01936	−0.03871	0.011988
G	0.05804	0.11608	0.107799
H	0.00708	0.01417	0.001606
AB + CF + DG	−0.00294	−0.00588	2.767E-04
AC + BF	−0.03103	−0.06206	0.030815
AD + BG	−0.18706	−0.37412	1.119705
AE	0.00402	0.00804	5.170E-04
AF + BC	−0.02251	−0.04502	0.016214
AG + BD	0.02644	0.05288	0.022370
AH	−0.02521	−0.05042	0.020339
BE	0.04925	0.09851	0.077627
BH	0.00654	0.01309	0.001371
CD + FG	0.01726	0.03452	0.009535
CE	0.01991	0.03982	0.012685
CG + DF	−0.00733	−0.01467	0.001721
CH	0.03040	0.06080	0.029568
DE	0.00854	0.01708	0.002334
DH	0.00784	0.01569	0.001969
EF	−0.00904	−0.01808	0.002616
EG	−0.02685	−0.05371	0.023078
EH	−0.01767	−0.03534	0.009993
FH	−0.01404	−0.02808	0.006308
GH	0.00245	0.00489	1.914E-04
ABE	0.01665	0.03331	0.008874
ABH	−0.00631	−0.01261	0.001273
ACD	−0.02717	−0.05433	0.023617

[a] Only main effects and two-factor interactions.

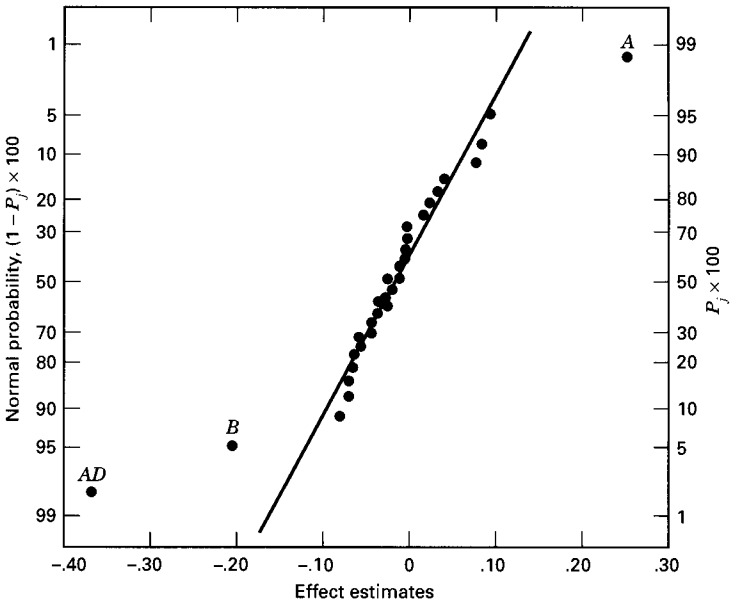


Figure 8-19 Normal probability plot of the effect estimates for Example 8-6.

the analysis following a log transformation. The effect estimates are shown in Table 8-17. Figure 8-19 is a normal probability plot of the effect estimates, using ln (standard deviation $\times$ 10^3) as the response variable. The only large effects are A = x-axis shift, B = y-axis shift, and the alias chain involving AD + BG. Now AD is the x-axis shift-tool vendor interaction, and BG is the y-axis shift-fixture height interaction, and since these two interactions are aliased it is impossible to separate them based on the data from the current experiment. Since both interactions involve one large main effect it is also difficult to apply any "obvious" simplifying logic to the situation either. If there is some engineering knowledge or process knowledge available that sheds light on the situation, then perhaps a choice could be made between the two interactions; otherwise, more data will be required to separate these two effects (the problem of adding runs to a fractional factorial to de-alias interactions is discussed in Section 8-5 and in the Supplemental Material for this chapter).

Suppose that process knowledge suggests that the appropriate interaction is likely to be AD. Table 8-18 is the resulting analysis of variance for the model with factors A, B,

Table 8-18 Analysis of Variance for Example 8-6

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
A	0.6740	1	0.6740	39.42	<0.0001
B	0.3217	1	0.3217	18.81	0.0002
D	0.0935	1	0.0935	5.47	0.0280
AD	1.1197	1	1.1197	65.48	<0.0001
Blocks	0.0201	3	0.0067		
Error	0.4099	24	0.0171		
Total	2.6389	31			

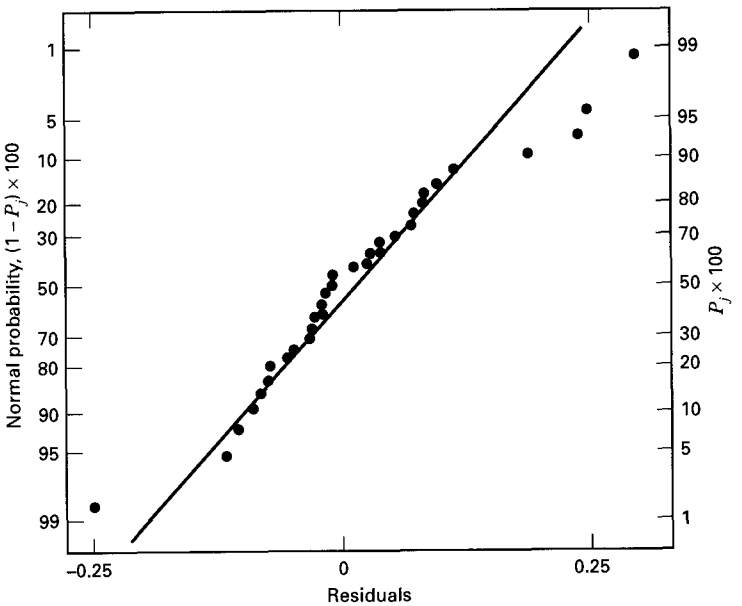


Figure 8-20 Normal probability plot of the residuals for Example 8-6.

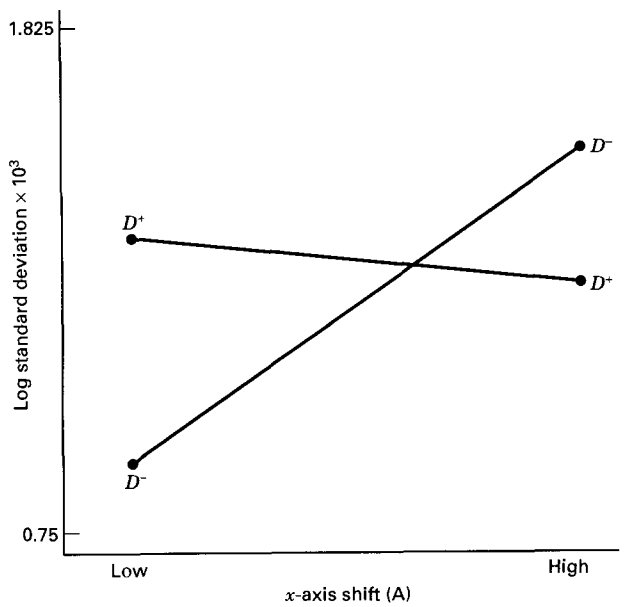


Figure 8-21 Plot of AD interaction for Example 8-6.

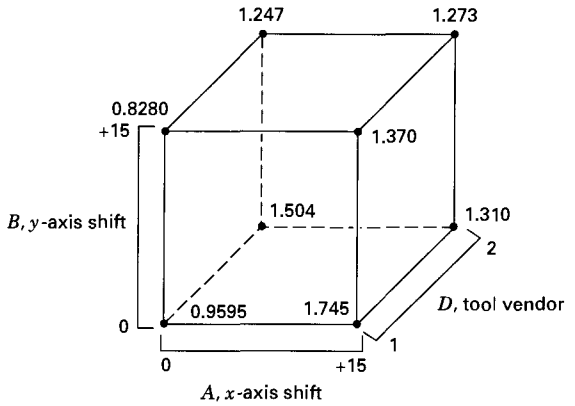


Figure 8-22 The 2_{IV}^{8-3} design in Example 8-6 projected into four replicates of a 2^3 design in factors A, B, and D.

D and AD (factor D was included to preserve the hierarchy principle). Notice that the block effect is small, suggesting that the machine spindles are not very different.

Figure 8-20 (on the facing page) is a normal probability plot of the residuals from this experiment. This plot is suggestive of slightly heavier than normal tails, so possibly other transformations should be considered. The AD interaction plot is in Figure 8-21 (on the facing page). Notice that tool vendor (D) and the magnitude of the x-axis shift (A) have a profound impact on the variability of the blade profile from design specifications. Running A at the low level (0 offset) and buying tools from vendor 1 gives the best results. Figure 8-22 shows the projection of this 2_{IV}^{8-3} design into four replicates of a 2^3 design in factors A, B, and D. The best combination of operating conditions is A at the low level (0 offset), B at the high level (0.015 in offset), and D at the low level (tool vendor 1).

8-5 RESOLUTION III DESIGNS

As indicated earlier, the sequential use of fractional factorial designs is very useful, often leading to great economy and efficiency in experimentation. We now illustrate these ideas using the class of resolution III designs.

It is possible to construct resolution III designs for investigating up to $k = N - 1$ factors in only N runs, where N is a multiple of 4. These designs are frequently useful in industrial experimentation. Designs in which N is a power of 2 can be constructed by the methods presented earlier in this chapter, and these are presented first. Of particular importance are designs requiring 4 runs for up to 3 factors, 8 runs for up to 7 factors and 16 runs for up to 15 factors. If $k = N - 1$, the fractional factorial design is said to be **saturated**.

A design for analyzing up to three factors in four runs is the 2_{III}^{3-1} design, presented in Section 8-2. Another very useful saturated fractional factorial is a design for studying seven factors in eight runs, that is, the 2_{III}^{7-4} design. This design is a one-sixteenth fraction of the 2^7. It may be constructed by first writing down as the basic design the plus and minus levels for a full 2^3 design in A, B, and C and then associating the levels of four additional factors with the interactions of the original three as follows: $D = AB$,

Table 8-19 The 2_{III}^{7-4} Design with the Generators $I = ABD$, $I = ACE$, $I = BCF$, and $I = ABCG$

	Basic Design							
Run	A	B	C	$D = AB$	$E = AC$	$F = BC$	$G = ABC$	
1	−	−	−	+	+	+	−	def
2	+	−	−	−	−	+	+	afg
3	−	+	−	−	+	−	+	beg
4	+	+	−	+	−	−	−	abd
5	−	−	+	+	−	−	+	cdg
6	+	−	+	−	+	−	−	ace
7	−	+	+	−	−	+	−	bcf
8	+	+	+	+	+	+	+	$abcdefg$

$E = AC$, $F = BC$, and $G = ABC$. Thus, the generators for this design are $I = ABD$, $I = ACE$, $I = BCF$, and $I = ABCG$. The design is shown in Table 8-19.

The complete defining relation for this design is obtained by multiplying the four generators ABD, ACE, BCF, and $ABCG$ together two at a time, three at a time, and four at a time, yielding

$$I = ABD = ACE = BCF = ABCG = BCDE = ACDF = CDG$$
$$= ABEF = BEG = AFG = DEF = ADEG = CEFG = BDFG = ABCDEFG$$

To find the aliases of any effect, simply multiply the effect by each word in the defining relation. For example, the aliases of B are

$$B = AD = ABCE = CF = ACG = CDE = ABCDF = BCDG = AEF = EG$$
$$= ABFG = BDEF = ABDEG = BCEFG = DFG = ACDEFG$$

This design is a one-sixteenth fraction, and because the signs chosen for the generators are positive, this is the principal fraction. It is also of resolution III because the smallest number of letters in any word of the defining contrast is three. Any one of the 16 different 2_{III}^{7-4} designs in this family could be constructed by using the generators with 1 of the 16 possible arrangements of signs in $I = \pm ABD$, $I = \pm ACE$, $I = \pm BCF$, $I = \pm ABCG$.

The seven degrees of freedom in this design may be used to estimate the seven main effects. Each of these effects has 15 aliases; however, if we assume that three-factor and higher interactions are negligible, then considerable simplification in the alias structure results. Making this assumption, each of the linear combinations associated with the seven main effects in this design actually estimates the main effect and three two-factor interactions:

$$\begin{aligned}
\ell_A &\rightarrow A + BD + CE + FG \\
\ell_B &\rightarrow B + AD + CF + EG \\
\ell_C &\rightarrow C + AE + BF + DG \\
\ell_D &\rightarrow D + AB + CG + EF \\
\ell_E &\rightarrow E + AC + BG + DF \\
\ell_F &\rightarrow F + BC + AG + DE \\
\ell_G &= G + CD + BE + AF
\end{aligned} \tag{8-1}$$

These aliases are found in Appendix Table XII(h), ignoring three-factor and higher interactions.

The saturated 2_{III}^{7-4} design in Table 8-19 can be used to obtain resolution III designs for studying fewer than seven factors in eight runs. For example, to generate a design for six factors in eight runs, simply drop any one column in Table 8-19, for example, column G. This produces the design shown in Table 8-20.

It is easy to verify that this design is also of resolution III; in fact, it is a 2_{III}^{6-3}, or a one-eighth fraction, of the 2^6 design. The defining relation for the 2_{III}^{6-3} design is equal to the defining relation for the original 2_{III}^{7-4} design with any words containing the letter G deleted. Thus, the defining relation for our new design is

$$I = ABD = ACE = BCF = BCDE = ACDF = ABEF = DEF$$

In general, when d factors are dropped to produce a new design, the new defining relation is obtained as those words in the original defining relation that do not contain any dropped letters. When constructing designs by this method, care should be exercised to obtain the best arrangement possible. If we drop columns B, D, F, and G from Table 8-19, we obtain a design for three factors in eight runs, yet the treatment combinations correspond to two replicates of a 2^3 design. The experimenter would probably prefer to run a full 2^3 design in A, C, and E.

It is also possible to obtain a resolution III design for studying up to 15 factors in 16 runs. This saturated 2_{III}^{15-11} design can be generated by first writing down the 16 treatment combinations associated with a 2^4 design in A, B, C, and D and then equating 11 new factors with the two-, three-, and four-factor interactions of the original four. In this design, each of the 15 main effects is aliased with seven two-factor interactions. A similar procedure can be used for the 2_{III}^{31-26} design, which allows up to 31 factors to be studied in 32 runs.

Sequential Assembly of Fractions to Separate Effects

By combining fractional factorial designs in which certain signs are switched, we can systematically isolate effects of potential interest. This type of sequential experiment is called a **fold over** of the original design. The alias structure for any fraction with the signs for one or more factors reversed is obtained by making changes of sign on the appropriate factors in the alias structure of the original fraction.

Consider the 2_{III}^{7-4} design in Table 8-19. Suppose that along with this principal frac-

Table 8-20 A 2_{III}^{6-3} Design with the Generators $I = ABD$, $I = ACE$, and $I = BCF$

	Basic Design						
Run	A	B	C	$D = AB$	$E = AC$	$F = BC$	
1	−	−	−	+	+	+	*def*
2	+	−	−	−	−	+	*af*
3	−	+	−	−	+	−	*be*
4	+	+	−	+	−	−	*abd*
5	−	−	+	+	−	−	*cd*
6	+	−	+	−	+	−	*ace*
7	−	+	+	−	−	+	*bcf*
8	+	+	+	+	+	+	*abcdef*

tion a second fractional design with the signs reversed in the column for factor D is also run. That is, the column for D in the second fraction is

$$-++--++-$$

The effects that may be estimated from the first fraction are shown in Equation 8-1, and from the second fraction we obtain

$$\begin{aligned}
\ell'_A &\rightarrow A - BD + CE + FG \\
\ell'_B &\rightarrow B - AD + CF + EG \\
\ell'_C &\rightarrow C + AE + BF - DG \\
\ell'_D &\rightarrow D - AB - CG - EF \\
\text{i.e.,} \quad \ell'_{-D} &\rightarrow -D + AB + CG + EF \qquad (8\text{-}2) \\
\ell'_E &\rightarrow E + AC + BG - DF \\
\ell'_F &\rightarrow F + BC + AG - DE \\
\ell'_G &\rightarrow G - CD + BE + AF
\end{aligned}$$

assuming that three-factor and higher interactions are insignificant. Now from the two linear combinations of effects $\frac{1}{2}(\ell_i + \ell'_i)$ and $\frac{1}{2}(\ell_i - \ell'_i)$ we obtain

i	From $\frac{1}{2}(\ell_i + \ell'_i)$	From $\frac{1}{2}(\ell_i - \ell'_i)$
A	$A + CE + FG$	BD
B	$B + CF + EG$	AD
C	$C + AE + BF$	DG
D	D	$AB + CG + EF$
E	$E + AC + BG$	DF
F	$F + BC + AG$	DE
G	$G + BE + AF$	CD

Thus, we have isolated the main effect of D and all of its two-factor interactions. In general, if we add to a fractional design of resolution III or higher a further fraction with the signs of a *single factor* reversed, then the combined design will provide estimates of the main effect of that factor and its two-factor interactions.

Now suppose we add to a resolution III fractional a second fraction in which the *signs for all the factors are reversed.* This type of fold over (sometimes called a **full fold over** or a reflection) breaks the alias links between main effects and two-factor interactions. That is, we may use the **combined design** to estimate all the main effects clear of any two-factor interactions. The following example illustrates the technique.

EXAMPLE 8-7

A human performance analyst is conducting an experiment to study eye focus time and has built an apparatus in which several factors can be controlled during the test. The factors he initially regards as important are acuity or sharpness of vision (A), distance from target to eye (B), target shape (C), illumination level (D), target size (E), target density (F), and subject (G). Two levels of each factor are considered. He suspects that only a few of these seven factors are of major importance and that high-order interactions between the factors can be neglected. On the basis of this assumption, the analyst decides

Table 8-21 A 2_{III}^{7-4} Design for the Eye Focus Time Experiment

	Basic Design								
Run	A	B	C	$D = AB$	$E = AC$	$F = BC$	$G = ABC$		Time
1	−	−	−	+	+	+	−	*def*	85.5
2	+	−	−	−	−	+	+	*afg*	75.1
3	−	+	−	−	+	−	+	*beg*	93.2
4	+	+	−	+	−	−	−	*abd*	145.4
5	−	−	+	+	−	−	+	*cdg*	83.7
6	+	−	+	−	+	−	−	*ace*	77.6
7	−	+	+	−	−	+	−	*bcf*	95.0
8	+	+	+	+	+	+	+	*abcdefg*	141.8

to run a screening experiment to identify the most important factors and then to concentrate further study on those. To screen these seven factors, he runs the treatment combinations from the 2_{III}^{7-4} design in Table 8-19 in random order, obtaining the focus times in milliseconds, as shown in Table 8-21.

Seven main effects and their aliases may be estimated from these data. From Equation 8-1, we see that the effects and their aliases are

$$\begin{aligned}
\ell_A &= 20.63 \rightarrow A + BD + CE + FG \\
\ell_B &= 38.38 \rightarrow B + AD + CF + EG \\
\ell_C &= -0.28 \rightarrow C + AE + BF + DG \\
\ell_D &= 28.88 \rightarrow D + AB + CG + EF \\
\ell_E &= -0.28 \rightarrow E + AC + BG + DF \\
\ell_F &= -0.63 \rightarrow F + BC + AG + DE \\
\ell_G &= -2.43 \rightarrow G + CD + BE + AF
\end{aligned}$$

For example,

$$\ell_A = \tfrac{1}{4}(-85.5 + 75.1 - 93.2 + 145.4 - 83.7 + 77.6 - 95.0 + 141.8) = 20.63$$

The three largest effects are ℓ_A, ℓ_B, and ℓ_D. The simplest interpretation of the data is that the main effects of A, B, and D are all significant. However, this interpretation is not unique, because one could also logically conclude that A, B, and the AB interaction, or perhaps B, D, and the BD interaction, or perhaps A, D, and the AD interaction are the true effects.

Notice that ABD is a word in the defining relation for this design. Therefore, this 2_{III}^{7-4} design does not project into a full 2^3 factorial in ABD; instead, it projects into two replicates of a 2^{3-1} design, as shown in Figure 8-23 (on the next page). Because the 2^{3-1} design is a resolution III design, A will be aliased with BD, B will be aliased with AD, and D will be aliased with AB, so the interactions cannot be separated from the main effects. The analyst here may have been unlucky. If he had assigned illumination level to C instead of D, the design would have projected into a full 2^3 design, and the interpretation could have been simpler.

To separate the main effects and the two-factor interactions, a second fraction is run with all the signs reversed. This fold-over design is shown in Table 8-22 (on the next page) along with the observed responses. Notice that when we fold over a resolution III

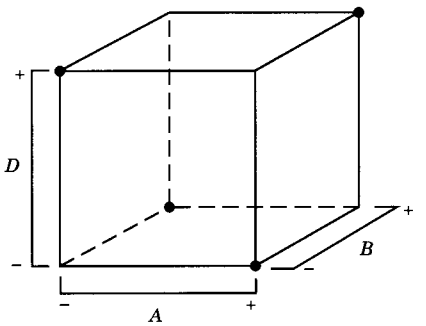


Figure 8-23 The 2^{7-4}_{III} design projected into two replicates of a 2^{3-1}_{III} design in A, B, and D.

design in this manner, we (in effect) change the signs on the generators that have an odd number of letters. The effects estimated by this fraction are

$$\begin{aligned}
\ell'_A &= -17.68 \rightarrow A - BD - CE - FG \\
\ell'_B &= 37.73 \rightarrow B - AD - CF - EG \\
\ell'_C &= -3.33 \rightarrow C - AE - BF - DG \\
\ell'_D &= 29.88 \rightarrow D - AB - CG - EF \\
\ell'_E &= 0.53 \rightarrow E - AC - BG - DF \\
\ell'_F &= 1.63 \rightarrow F - BC - AG - DE \\
\ell'_G &= 2.68 \rightarrow G - CD - BE - AF
\end{aligned}$$

By combining this second fraction with the original one, we obtain the following estimates of the effects:

i	From $\frac{1}{2}(\ell_i + \ell'_i)$	From $\frac{1}{2}(\ell_i - \ell'_i)$
A	$A = 1.48$	$\boldsymbol{BD} + CE + FG = 19.15$
B	$\boldsymbol{B} = 38.05$	$AD + CF + EG = 0.33$
C	$C = -1.80$	$AE + BF + DG = 1.53$
D	$\boldsymbol{D} = 29.38$	$AB + CG + EF = -0.50$
E	$E = 0.13$	$AC + BG + DF = -0.40$
F	$F = 0.50$	$BC + AG + DE = -1.53$
G	$G = 0.13$	$CD + BE + AF = -2.55$

Table 8-22 A Fold-Over 2^{7-4}_{III} Design for the Eye Focus Time Experiment

	Basic Design								
Run	A	B	C	$D = -AB$	$E = -AC$	$F = -BC$	$G = ABC$		Time
1	+	+	+	−	−	−	+	*abcg*	91.3
2	−	+	+	+	+	−	−	*bcde*	136.7
3	+	−	+	+	−	+	−	*acdf*	82.4
4	−	−	+	−	+	+	+	*cefg*	73.4
5	+	+	−	−	+	+	−	*abef*	94.1
6	−	+	−	+	−	+	+	*bdfg*	143.8
7	+	−	−	+	+	−	+	*adeg*	87.3
8	−	−	−	−	−	−	−	(1)	71.9

The two largest effects are B and D. Furthermore, the third largest effect is $BD + CE + FG$, so it seems reasonable to attribute this to the BD interaction. The analyst used the two factors distance (B) and illumination level (D) in subsequent experiments with the other factors A, C, E, and F at standard settings and verified the results obtained here. He decided to use subjects as blocks in these new experiments rather than ignore a potential subject effect because several different subjects had to be used to complete the experiment.

The Defining Relation for a Fold-Over Design

Combining fractional factorial designs via fold over as demonstrated in Example 8-7 is a very useful technique. It is often of interest to know the defining relation for the combined design. It can be easily determined. Each separate fraction will have $L + U$ words used as generators: L words of like sign and U words of unlike sign. The combined design will have $L + U - 1$ words used as generators. These will be the L words of like sign and the $U - 1$ words consisting of independent even products of the words of unlike sign. (**Even products** are words taken two at a time, four at a time, and so forth.)

To illustrate this procedure, consider the design in Example 8-7. For the first fraction, the generators are

$$I = ABD, \quad I = ACE, \quad I = BCF, \quad \text{and} \quad I = ABCG$$

and for the second fraction, they are

$$I = -ABD, \quad I = -ACE, \quad I = -BCF, \quad \text{and} \quad I = ABCG$$

Notice that in the second fraction we have switched the signs on the generators with an odd number of letters. Also, notice that $L + U = 1 + 3 = 4$. The combined design will have $I = ABCG$ (the like sign word) as a generator and two words that are independent even products of the words of unlike sign. For example, take $I = ABD$ and $I = ACE$; then $I = (ABD)(ACE) = BCDE$ is a generator of the combined design. Also, take $I = ABD$ and $I = BCF$; then $I = (ABD)(BCF) = ACDF$ is a generator of the combined design. The complete defining relation for the combined design is

$$I = ABCG = BCDE = ACDF = ADEG = BDFG = ABEF = CEFG$$

Plackett–Burman Designs

These designs, attributed to Plackett and Burman (1946), are two-level fractional factorial designs for studying $k = N - 1$ variables in N runs, where N is a multiple of 4. If N is a power of 2, these designs are identical to those presented earlier in this section. However, for $N = 12$, 20, 24, 28, and 36, the Plackett–Burman designs are sometimes of interest. Because these designs cannot be represented as cubes, they are sometimes called **nongeometric designs**.

The upper half of Table 8-23 (on the next page) presents rows of plus and minus signs that are used to construct the Plackett–Burman designs for $N = 12$, 20, 24, and 36, whereas the lower half of the table presents blocks of plus and minus signs for constructing the design for $N = 28$. The designs for $N = 12$, 20, 24, and 36 are obtained by writing the appropriate row in Table 8-23 as a column (or row). A second column (or row) is then generated from this first one by moving the elements of the column (or row) down (or to the right) one position and placing the last element in the first position. A third column (or row) is produced from the second similarly, and the process is continued

Table 8-23 Plus and Minus Signs for the Plackett–Burman Designs

$k = 11, N = 12$ ++−+++−−−+−
$k = 19, N = 20$ ++−−++++−+−+−−−−++−
$k = 23, N = 24$ +++++−+−++−−++−−+−+−−−−
$k = 35, N = 36$ −+−+++−−−+++++−+++−−+−−−−+−+−++−−+−

$k = 27, N = 28$

+−++++−−−	−+−−−+−−+	++−+−++−+
++−+++−−−	−−+−−+−−	−++++−++−
−++++−−−	+−−−+−−+−	+−+−++−++
−−−+−++++	−−+−+−−−+	+−+++−+−+
−−−++−+++	+−−−−++−−	++−−++++−
−−−−+++++	−+−+−−−+−	−+++−+−++
+++−−−+−+	−−+−−+−+−	+−++−+++−
+++−−−++−	+−−+−−−−+	++−++−−++
+++−−−−++	−+−−+−+−−	−++−+++−+

until column (or row) k is generated. A row of minus signs is then added, completing the design. For $N = 28$, the three blocks X, Y, and Z are written down in the order

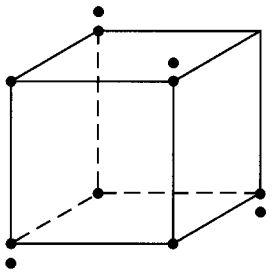
$$\begin{matrix} X & Y & Z \\ Z & X & Y \\ Y & Z & X \end{matrix}$$

and a row of minus signs is added to these 27 rows. The design for $N = 12$ runs and $k = 11$ factors is shown in Table 8-24.

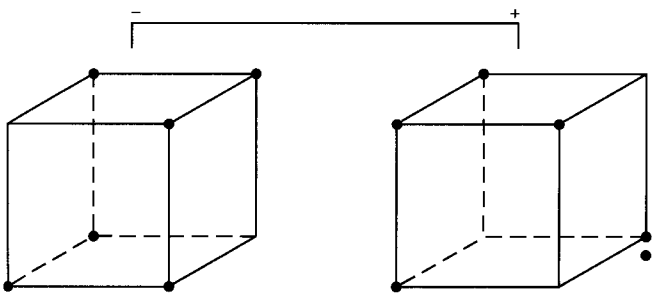
The nongeometric Plackett–Burman designs for $N = 12$, 20, 24, 28, and 36 have very messy alias structures. For example, in the 12-run design every main effect is **partially aliased** with every two-factor interaction not involving itself. For example, the AB interaction is aliased with the nine main effects $C, D, \ldots, K$. Furthermore, each main effect is **partially aliased** with 45 two-factor interactions. In the larger designs, the situation is even more complex. We advise the experimenter to use these designs *very carefully*.

Table 8-24 Plackett–Burman Design for $N = 12$, $k = 11$

Run	A	B	C	D	E	F	G	H	I	J	K
1	+	−	+	−	−	−	+	+	+	−	+
2	+	+	−	+	−	−	−	+	+	+	−
3	−	+	+	−	+	−	−	−	+	+	+
4	+	−	+	+	−	+	−	−	−	+	+
5	+	+	−	+	+	−	+	−	−	−	+
6	+	+	+	−	+	+	−	+	−	−	−
7	−	+	+	+	−	+	+	−	+	−	−
8	−	−	+	+	+	−	+	+	−	+	−
9	−	−	−	+	+	+	−	+	+	−	+
10	+	−	−	−	+	+	+	−	+	+	−
11	−	+	−	−	−	+	+	+	−	+	+
12	−	−	−	−	−	−	−	−	−	−	−



(*a*) Projection into three factors



(*b*) Projection into four factors

Figure 8-24 Projection of the 12-run Plackett–Burman design into three- and four-factor designs.

The projective properties of the nongeometric Plackett–Burman designs are not terribly attractive. For example, consider the 12-run design in Table 8-24. This design will project into three replicates of a full 2^2 design in any two of the original 11 factors. However, in three factors, the projected design is a full 2^3 factorial plus a 2_{III}^{3-1} fractional factorial (see Figure 8-24*a*). Thus, the resolution III Plackett–Burman design has **projectivity** 3, meaning it will collapse into a full factorial in any subset of three factors. The 2_{III}^{k-p} design only has projectivity 2. The four-dimensional projections are shown in Figure 8-24*b*. Notice that these three- and four-factor projections are not balanced designs.

EXAMPLE 8-8

We will illustrate some of the potential difficulties associated with the Plackett–Burman designs by using the 11-variable, 12-run design and a set of simulated data. We will assume that the process has three significant main effects (A, B, D) and two significant two-factor interactions (AB and AD). The model is

$$y = 200 + 8x_1 + 10x_2 + 12x_4 - 12x_1x_2 + 9x_1x_4 + \epsilon$$

where each x_i is a coded variable defined on the -1, $+1$ interval and ϵ is an NID(0, 9) random error term. Therefore, three of the $k = 11$ factors are large, and there are two large interactions; not an unreasonable situation.

Table 8-25 (page 346) presents the 12-run Plackett–Burman design and the simulated responses. This design looks different from the 12-run design in Table 8-24 because it

Table 8-25 Plackett–Burman Design for Example 8-8

Run	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*	*J*	*K*	*L*	Response
1	+	+	−	+	+	+	−	−	−	+	−	231
2	−	+	+	−	+	+	+	−	−	−	+	207
3	+	−	+	+	−	+	+	+	−	−	−	230
4	−	+	−	+	+	−	+	+	+	−	−	217
5	−	−	+	−	+	+	−	+	+	+	−	175
6	−	−	−	+	−	+	+	−	+	+	+	176
7	+	−	−	−	+	−	+	+	−	+	+	183
8	+	+	−	−	−	+	−	+	+	−	+	185
9	+	+	+	−	−	−	+	−	+	+	−	181
10	−	+	+	+	−	−	−	+	−	+	+	220
11	+	−	+	+	+	−	−	−	+	−	+	229
12	−	−	−	−	−	−	−	−	−	−	−	168

was constructed using the row of signs for $k = 11, N = 12$ in Table 8-23 as a row. The effect estimates are shown in Table 8-26. Notice that there are seven large effects; *A*, *B*, *C*, *D*, *E*, *J*, and *K* (and, of course, their aliases). It is not immediately obvious that some of these effects could be interactions. Some of this ambiguity could be resolved by folding over the design. This will generally resolve the main effects, but it often still leaves the experimenter uncertain about interaction effects.

The difficulty in interpretation in a Plackett–Burman design, illustrated in the above example, occurs fairly often in practice. If your choice is between a geometric 2_{III}^{11-7} design with 16 runs or a 12-run Plackett–Burman design that may have to be folded over (thereby requiring 24 runs), the geometric design may turn out to be a better choice. For more details, see Montgomery, Borror, and Stanley (1997–98). Under some conditions,

Table 8-26 Effect Estimates, Regression Coefficients, and Sums of Squares for Example 8-8

Variable[a]	Regression Coefficient	Estimated Effect	Sum of Squares
Overall Average	200.167		
A	6.333	12.667	481.333
B	6.667	13.333	533.333
C	6.833	12.667	560.333
D	17.000	34.000	3468.000
E	6.833	13.667	560.333
F	0.500	1.000	3.000
G	−1.167	−2.333	16.333
H	1.500	3.000	27.000
J	−6.333	−12.667	481.333
K	−5.833	−11.667	408.333
L	−0.167	−0.333	0.333

[a] Every main effect is partially aliased with 45 two-factor interactions.

we can untangle the aliases in a nongeometric Plackett–Burman design by using regression model-building techniques. This is discussed by Hamada and Wu (1992).

8-6 RESOLUTION IV AND V DESIGNS

A 2^{k-p} fractional factorial design is of resolution IV if the main effects are clear of two-factor interactions and some two-factor interactions are aliased with each other. Thus, if three-factor and higher interactions are suppressed, the main effects may be estimated directly in a 2^{k-p}_{IV} design. An example is the 2^{6-2}_{IV} design in Table 8-10. Furthermore, the two combined fractions of the 2^{7-4}_{III} design in Example 8-7 yields a 2^{7-3}_{IV} design.

Any 2^{k-p}_{IV} design must contain at least $2k$ runs. Resolution IV designs that contain exactly $2k$ runs are called **minimal designs**. Resolution IV designs may be obtained from resolution III designs by the process of **fold over**. Recall that to fold over a 2^{k-p}_{III} design, simply add to the original fraction a second fraction with all the signs reversed. Then the plus signs in the identity column I in the first fraction could be switched in the second fraction, and a $(k + 1)$st factor could be associated with this column. The result is a 2^{k+1-p}_{IV} fractional factorial design. The process is demonstrated in Table 8-27 for the 2^{3-1}_{III} design. It is easy to verify that the resulting design is a 2^{4-1}_{IV} design with defining relation $I = ABCD$.

It is also possible to fold over resolution IV designs to separate two-factor interactions that are aliased with each other. Montgomery and Runger (1996) observe that an experimenter may have several objectives in folding over a resolution IV design, such as (1) break as many two-factor interaction alias chains as possible, (2) break the two-factor interactions on a specific alias chain, or (3) break the two-factor interactions involving a specific factor. One way to fold over a resolution IV design is to run a second fraction in which the sign is reversed on every design generator that has an even number of letters. To illustrate, consider the 2^{6-2}_{IV} design used for the injection molding experiment in Example 8-4. The generators for the design in Table 8-10 are $I = ABCE$ and $I = BCDF$. The second fraction would use the generators $I = -ABCE$ and $I = -BCDF$, and

Table 8-27 A 2^{4-1}_{IV} Design Obtained by Fold Over

D			
I	A	B	C
Original 2^{3-1}_{III} $I = ABC$			
+	−	−	+
+	+	−	−
+	−	+	−
+	+	+	+
Second 2^{3-1}_{III} with Signs Switched			
−	+	+	−
−	−	+	+
−	+	−	+
−	−	−	−

the single generator for the combined design would be $I = ADEF$. Thus, the combined design is still a resolution IV fractional factorial design. However, the alias relationships will be much simpler than in the original 2_{IV}^{6-2} design. In fact, the only two-factor interactions that will be aliased are $AD = EF$, $AE = DF$, and $AF = DE$. All the other two-factor interactions can be estimated from the combined design.

As another example, consider the 2_{IV}^{8-3} design with 32 runs. Table 8-14 indicates that the best set of generators for this design is $I = ABCF$, $I = ABDG$, and $I = BCDEH$. Appendix Table XII(m) shows the aliases for this design. Notice that there are six pairs of two-factor interactions and one group of three two-factor interactions that are aliases. If we fold over this design, the second fraction would have the generators $I = -ABCF$, $I = -ABDG$, and $I = BCDEH$. The combined design has the generators $I = CDFG$ and $I = BCDEH$, and the complete defining relation is

$$I = CDFG = BCDEH = BEFGH$$

The combined design is of resolution IV, but the only two-factor interactions that are still aliased are $CD = FG$, $CF = DG$, and $CG = DF$. This is a considerable simplification of the aliasing in the original fraction.

Notice that when we start with a resolution III design, the fold-over procedure guarantees that the combined design will be of resolution IV, thereby ensuring that all the main effects can be separated from their two-factor interaction aliases. When folding over a resolution IV design, we will not necessarily separate *all* the two-factor interactions. In fact, if the *original* fraction has an alias structure with more than two two-factor interactions in any alias chain, folding over will not completely separate all the two-factor interactions. Both of the foregoing examples, the 2_{IV}^{6-2} and the 2_{IV}^{8-3}, have at least one such two-factor interaction alias chain. Montgomery and Runger (1996) give a table of recommended fold-over designs for resolution IV fractions with $6 \leq k \leq 10$ factors.

Resolution V designs are fractional factorials in which the main effects and the two-factor interactions do not have other main effects and two-factor interactions as their aliases. These are very powerful designs, allowing the unique estimation of all the main effects and two-factor interactions, provided that all the three-factor and higher interactions are negligible. The smallest word in the defining relation of such a design must have five letters. The 2^{5-1} design with the generating relation $I = ABCDE$ is of resolution V. Another example is the 2_{V}^{8-2} design with the generating relations $I = ABCDG$ and $I = ABEFH$. Further examples of these designs are given by Box and Hunter (1961b).

Because the standard resolution V designs are large designs when the number of factors is moderately large, there is some practical interest in irregular resolution V fractional factorials. These are useful designs for $4 \leq k \leq 9$ factors. The 24-run design for $k = 5$ factors is shown in Table 8-28. Because this is a resolution V design, all five main effects and all 10 two-factor interactions can be estimated, assuming that three-factor and higher interactions are negligible. The design for $k = 4$ factors has 12 runs and is discussed in Problem 8-22. For $k = 6$, 7, and 8 these designs have 48 runs, and the nine-factor design has 96 runs. The Design-Expert software package contains all of these designs.

Finally, we point out that a complete fold over of a resolution IV or V design is usually unnecessary. Generally, there are only one or two (or a very few) aliased interactions that are potentially of interest. These interactions can usually be de-aliased by adding a smaller number of runs to the original fraction. This technique is sometimes

Table 8-28 The Irregular Resolution V Fraction for Five Factors in 24 Runs

A	B	C	D	E
−	−	−	−	−
−	+	−	−	−
+	+	−	−	−
−	−	+	−	−
+	−	+	−	−
−	+	+	−	−
−	−	−	+	−
+	−	−	+	−
+	+	−	+	−
+	−	+	+	−
−	+	+	+	−
+	+	+	+	−
−	−	−	−	+
+	−	−	−	+
+	+	−	−	+
+	−	+	−	+
−	+	+	−	+
+	+	+	−	+
−	−	−	+	+
−	+	−	+	+
+	+	−	+	+
−	−	+	+	+
+	−	+	+	+
−	+	+	+	+

called a **partial fold over**. Refer to Example 10-5 and the supplemental text material for this chapter for some insight regarding how this is done.

8-7 SUMMARY

This chapter has introduced the 2^{k-p} fractional factorial design. We have emphasized the use of these designs in screening experiments to quickly and efficiently identify the subset of factors that are active and to provide some information on interaction. The projective property of these designs makes it possible in many cases to examine the active factors in more detail. Sequential assembly of these designs via fold over is a very effective way to gain additional information about interactions that an initial experiment may identify as possibly important.

In practice, 2^{k-p} fractional factorial designs with $N = 4$, 8, 16, and 32 runs are highly useful. Table 8-29 (page 350) summarizes these designs, identifying how many factors can be used with each design to obtain various types of screening experiments. For example, the 16-run design is a full factorial for 4 factors, a one-half fraction for 5 factors, a resolution IV fraction for 6 to 8 factors, and a resolution III fraction for 9 to 15 factors. All of these designs may be constructed using the methods discussed in this chapter, and many of their alias structures are shown in Appendix Table XII.

Table 8-29 Useful Factorial and Fractional Factorial Designs from the 2^{k-p} System. The Numbers in the Cells are the Number of Factors in the Experiment

	Number of Runs			
Design Type	4	8	16	32
Full factorial	2	3	4	5
Half-fraction	3	4	5	6
Resolution IV fraction	—	4	6–8	7–16
Resolution III fraction	3	5–7	9–15	17–31

8-8 PROBLEMS

8-1. Suppose that in the chemical process development experiment described in Problem 6-7, it was only possible to run a one-half fraction of the 2^4 design. Construct the design and perform the statistical analysis, using the data from replicate I.

8-2. Suppose that in Problem 6-15, only a one-half fraction of the 2^4 design could be run. Construct the design and perform the analysis, using the data from replicate I.

8-3. Consider the plasma etch experiment described in Problem 6-18. Suppose that only a one-half fraction of the design could be run. Set up the design and analyze the data.

8-4. Problem 6-21 describes a process improvement study in the manufacturing process of an integrated circuit. Suppose that only eight runs could be made in this process. Set up an appropriate 2^{5-2} design and find the alias structure. Use the appropriate observations from Problem 6-21 as the observations in this design and estimate the factor effects. What conclusions can you draw?

8-5. ***Continuation of Problem 8-4.*** Suppose you have made the eight runs in the 2^{5-2} design in Problem 8-4. What additional runs would be required to identify the factor effects that are of interest? What are the alias relationships in the combined design?

8-6. R. D. Snee ("Experimenting with a Large Number of Variables," in *Experiments in Industry: Design, Analysis and Interpretation of Results*, by R. D. Snee, L. B. Hare, and J. B. Trout, Editors, ASQC, 1985) describes an experiment in which a 2^{5-1} design with $I = ABCDE$ was used to investigate the effects of five factors on the color of a chemical product. The factors are A = solvent/reactant, B = catalyst/reactant, C = temperature, D = reactant purity, and E = reactant pH. The results obtained were as follows:

e	-0.63	d	6.79
a	2.51	ade	5.47
b	-2.68	bde	3.45
abe	1.66	abd	5.68
c	2.06	cde	5.22
ace	1.22	acd	4.38
bce	-2.09	bcd	4.30
abc	1.93	$abcde$	4.05

(a) Prepare a normal probability plot of the effects. Which effects seem active?

(b) Calculate the residuals. Construct a normal probability plot of the residuals and plot the residuals versus the fitted values. Comment on the plots.

(c) If any factors are negligible, collapse the 2^{5-1} design into a full factorial in the active factors. Comment on the resulting design, and interpret the results.

8-7. An article by J. J. Pignatiello, Jr. and J. S. Ramberg in the *Journal of Quality Technology* (Vol. 17, 1985, pp. 198–206) describes the use of a replicated fractional factorial to investigate the effect of five factors on the free height of leaf springs used in an automotive

application. The factors are A = furnace temperature, B = heating time, C = transfer time, D = hold down time, and E = quench oil temperature. The data are shown below:

A	B	C	D	E	Free Height		
−	−	−	−	−	7.78	7.78	7.81
+	−	−	+	−	8.15	8.18	7.88
−	+	−	+	−	7.50	7.56	7.50
+	+	−	−	−	7.59	7.56	7.75
−	−	+	+	−	7.54	8.00	7.88
+	−	+	−	−	7.69	8.09	8.06
−	+	+	−	−	7.56	7.52	7.44
+	+	+	+	−	7.56	7.81	7.69
−	−	−	−	+	7.50	7.25	7.12
+	−	−	+	+	7.88	7.88	7.44
−	+	−	+	+	7.50	7.56	7.50
+	+	−	−	+	7.63	7.75	7.56
−	−	+	+	+	7.32	7.44	7.44
+	−	+	−	+	7.56	7.69	7.62
−	+	+	−	+	7.18	7.18	7.25
+	+	+	+	+	7.81	7.50	7.59

(a) Write out the alias structure for this design. What is the resolution of this design?
(b) Analyze the data. What factors influence the mean free height?
(c) Calculate the range and standard deviation of the free height for each run. Is there any indication that any of these factors affects variability in the free height?
(d) Analyze the residuals from this experiment, and comment on your findings.
(e) Is this the best possible design for five factors in 16 runs? Specifically, can you find a fractional design for five factors in 16 runs with a higher resolution than this one?

8-8. An article in *Industrial and Engineering Chemistry* ("More on Planning Experiments to Increase Research Efficiency," 1970, pp. 60–65) uses a 2^{5-2} design to investigate the effect of A = condensation temperature, B = amount of material 1, C = solvent volume, D = condensation time, and E = amount of material 2 on yield. The results obtained are as follows:

$e = 23.2$	$ad = 16.9$	$cd = 23.8$	$bde = 16.8$
$ab = 15.5$	$bc = 16.2$	$ace = 23.4$	$abcde = 18.1$

(a) Verify that the design generators used were $I = ACE$ and $I = BDE$.
(b) Write down the complete defining relation and the aliases for this design.
(c) Estimate the main effects.
(d) Prepare an analysis of variance table. Verify that the AB and AD interactions are available to use as error.
(e) Plot the residuals versus the fitted values. Also construct a normal probability plot of the residuals. Comment on the results.

8-9. Consider the leaf spring experiment in Problem 8-7. Suppose that factor E (quench oil temperature) is very difficult to control during manufacturing. Where would you set factors A, B, C, and D to reduce variability in the free height as much as possible regardless of the quench oil temperature used?

8-10. Construct a 2^{7-2} design by choosing two four-factor interactions as the independent generators. Write down the complete alias structure for this design. Outline the analysis of variance table. What is the resolution of this design?

8-11. Consider the 2^5 design in Problem 6-21. Suppose that only a one-half fraction could be run. Furthermore, two days were required to take the 16 observations, and it was necessary to confound the 2^{5-1} design in two blocks. Construct the design and analyze the data.

8-12. Analyze the data in Problem 6-23 as if it came from a 2^{4-1}_{IV} design with $I = ABCD$. Project the design into a full factorial in the subset of the original four factors that appear to be significant.

8-13. Repeat Problem 8-12 using $I = -ABCD$. Does use of the alternate fraction change your interpretation of the data?

8-14. Project the 2^{4-1}_{IV} design in Example 8-1 into two replicates of a 2^2 design in the factors A and B. Analyze the data and draw conclusions.

8-15. Construct a 2^{6-3}_{III} design. Determine the effects that may be estimated if a second fraction of this design is run with all signs reversed.

8-16. Consider the 2^{6-3}_{III} design in Problem 8-15. Determine the effects that may be estimated if a second fraction of this design is run with the signs for factor A reversed.

8-17. Fold over the 2^{7-4}_{III} design in Table 8-19 to produce an eight-factor design. Verify that the resulting design is a 2^{8-4}_{IV} design. Is this a minimal design?

8-18. Fold over a 2^{5-2}_{III} design to produce a six-factor design. Verify that the resulting design is a 2^{6-2}_{IV} design. Compare this design to the 2^{6-2}_{IV} design in Table 8-10.

8-19. An industrial engineer is conducting an experiment using a Monte Carlo simulation model of an inventory system. The independent variables in her model are the order quantity (A), the reorder point (B), the setup cost (C), the backorder cost (D), and the carrying cost rate (E). The response variable is average annual cost. To conserve computer time, she decides to investigate these factors using a 2^{5-2}_{III} design with $I = ABD$ and $I = BCE$. The results she obtains are $de = 95$, $ae = 134$, $b = 158$, $abd = 190$, $cd = 92$, $ac = 187$, $bce = 155$, and $abcde = 185$.

(a) Verify that the treatment combinations given are correct. Estimate the effects, assuming three-factor and higher interactions are negligible.

(b) Suppose that a second fraction is added to the first, for example, $ade = 136$, $e = 93$, $ab = 187$, $bd = 153$, $acd = 139$, $c = 99$, $abce = 191$, and $bcde = 150$. How was this second fraction obtained? Add this data to the original fraction, and estimate the effects.

(c) Suppose that the fraction $abc = 189$, $ce = 96$, $bcd = 154$, $acde = 135$, $abe = 193$, $bde = 152$, $ad = 137$, and $(1) = 98$ was run. How was this fraction obtained? Add this data to the original fraction and estimate the effects.

8-20. Construct a 2^{5-1} design. Show how the design may be run in two blocks of eight observations each. Are any main effects or two-factor interactions confounded with blocks?

8-21. Construct a 2^{7-2} design. Show how the design may be run in four blocks of eight observations each. Are any main effects or two-factor interactions confounded with blocks?

8-22. ***Irregular fractions of the 2^k [John (1971)].*** Consider a 2^4 design. We must estimate the four main effects and the six two-factor interactions, but the full 2^4 factorial cannot be run. The largest possible block size contains 12 runs. These 12 runs can be obtained from the four one-quarter replicates defined by $I = \pm AB = \pm ACD = \pm BCD$ by omitting the principal fraction. Show how the remaining three 2^{4-2} fractions can be combined to estimate the required effects, assuming three-factor and higher interactions are negligible. This design could be thought of as a three-quarter fraction.

8-23. Carbon anodes used in a smelting process are baked in a ring furnace. An experiment is run in the furnace to determine which factors influence the weight of packing material that is stuck to the anodes after baking. Six variables are of interest, each at two levels: A = pitch/fines ratio (0.45, 0.55), B = packing material type (1, 2), C = packing material temperature (ambient, 325°C), D = flue location (inside, outside), E = pit temperature (ambient, 195°C), and F = delay time before packing (zero, 24 hours). A 2^{6-3} design is

run, and three replicates are obtained at each of the design points. The weight of packing material stuck to the anodes is measured in grams. The data in run order are as follows: *abd* = (984, 826, 936); *abcdef* = (1275, 976, 1457); *be* = (1217, 1201, 890); *af* = (1474, 1164, 1541); *def* = (1320, 1156, 913); *cd* = (765, 705, 821); *ace* = (1338, 1254, 1294); and *bcf* = (1325, 1299, 1253). We wish to minimize the amount of stuck packing material.

(a) Verify that the eight runs correspond to a 2_{III}^{6-3} design. What is the alias structure?

(b) Use the average weight as a response. What factors appear to be influential?

(c) Use the range of the weights as a response. What factors appear to be influential?

(d) What recommendations would you make to the process engineers?

8-24. A 16-run experiment was performed in a semiconductor manufacturing plant to study the effects of six factors on the curvature or camber of the substrate devices produced. The six variables and their levels are shown below:

Run	Lamination Temperature (°C)	Lamination Time (s)	Lamination Pressure (tn)	Firing Temperature (°C)	Firing Cycle Time (h)	Firing Dew Point (°C)
1	55	10	5	1580	17.5	20
2	75	10	5	1580	29	26
3	55	25	5	1580	29	20
4	75	25	5	1580	17.5	26
5	55	10	10	1580	29	26
6	75	10	10	1580	17.5	20
7	55	25	10	1580	17.5	26
8	75	25	10	1580	29	20
9	55	10	5	1620	17.5	26
10	75	10	5	1620	29	20
11	55	25	5	1620	29	26
12	75	25	5	1620	17.5	20
13	55	10	10	1620	29	20
14	75	10	10	1620	17.5	26
15	55	25	10	1620	17.5	20
16	75	25	10	1620	29	26

Each run was replicated four times, and a camber measurement was taken on the substrate. The data are shown below:

Run	Camber for Replicate (in/in)				Total (10^{-4} in/in)	Mean (10^{-4} in/in)	Standard Deviation
	1	2	3	4			
1	0.0167	0.0128	0.0149	0.0185	629	157.25	24.418
2	0.0062	0.0066	0.0044	0.0020	192	48.00	20.976
3	0.0041	0.0043	0.0042	0.0050	176	44.00	4.083
4	0.0073	0.0081	0.0039	0.0030	223	55.75	25.025
5	0.0047	0.0047	0.0040	0.0089	223	55.75	22.410
6	0.0219	0.0258	0.0147	0.0296	920	230.00	63.639
7	0.0121	0.0090	0.0092	0.0086	389	97.25	16.029
8	0.0255	0.0250	0.0226	0.0169	900	225.00	39.42
9	0.0032	0.0023	0.0077	0.0069	201	50.25	26.725
10	0.0078	0.0158	0.0060	0.0045	341	85.25	50.341

Run	Camber for Replicate (in/in) 1	2	3	4	Total (10^{-4} in/in)	Mean (10^{-4} in/in)	Standard Deviation
11	0.0043	0.0027	0.0028	0.0028	126	31.50	7.681
12	0.0186	0.0137	0.0158	0.0159	640	160.00	20.083
13	0.0110	0.0086	0.0101	0.0158	455	113.75	31.12
14	0.0065	0.0109	0.0126	0.0071	371	92.75	29.51
15	0.0155	0.0158	0.0145	0.0145	603	150.75	6.75
16	0.0093	0.0124	0.0110	0.0133	460	115.00	17.45

(a) What type of design did the experimenters use?
(b) What are the alias relationships in this design?
(c) Do any of the process variables affect average camber?

Table 8-30 Data for Problem 8-25

Run	*A* Volume	*B* Batch	*C* Time, s	*D* Speed	*E* Acc.	*F* Cover	Resist Thickness Left	Center	Right	Avg.	Range
1	5	Batch 2	14	7350	5	Off	4531	4531	4515	4525.7	16
2	5	Batch 1	6	7350	5	Off	4446	4464	4428	4446	36
3	3	Batch 1	6	6650	5	Off	4452	4490	4452	4464.7	38
4	3	Batch 2	14	7350	20	Off	4316	4328	4308	4317.3	20
5	3	Batch 1	14	7350	5	Off	4307	4295	4289	4297	18
6	5	Batch 1	6	6650	20	Off	4470	4492	4495	4485.7	25
7	3	Batch 1	6	7350	5	On	4496	4502	4482	4493.3	20
8	5	Batch 2	14	6650	20	Off	4542	4547	4538	4542.3	9
9	5	Batch 1	14	6650	5	Off	4621	4643	4613	4625.7	30
10	3	Batch 1	14	6650	5	On	4653	4670	4645	4656	25
11	3	Batch 2	14	6650	20	On	4480	4486	4470	4478.7	16
12	3	Batch 1	6	7350	20	Off	4221	4233	4217	4223.7	16
13	5	Batch 1	6	6650	5	On	4620	4641	4619	4626.7	22
14	3	Batch 1	6	6650	20	On	4455	4480	4466	4467	25
15	5	Batch 2	14	7350	20	On	4255	4288	4243	4262	45
16	5	Batch 2	6	7350	5	On	4490	4534	4523	4515.7	44
17	3	Batch 2	14	7350	5	On	4514	4551	4540	4535	37
18	3	Batch 1	14	6650	20	Off	4494	4503	4496	4497.7	9
19	5	Batch 2	6	7350	20	Off	4293	4306	4302	4300.3	13
20	3	Batch 2	6	7350	5	Off	4534	4545	4512	4530.3	33
21	5	Batch 1	14	6650	20	On	4460	4457	4436	4451	24
22	3	Batch 2	6	6650	5	On	4650	4688	4656	4664.7	38
23	5	Batch 1	14	7350	20	Off	4231	4244	4230	4235	14
24	3	Batch 2	6	7350	20	On	4225	4228	4208	4220.3	20
25	5	Batch 1	14	7350	5	On	4381	4391	4376	4382.7	15
26	3	Batch 2	6	6650	20	Off	4533	4521	4511	4521.7	22
27	3	Batch 1	14	7350	20	On	4194	4230	4172	4198.7	58
28	5	Batch 2	6	6650	5	Off	4666	4695	4672	4677.7	29
29	5	Batch 1	6	7350	20	On	4180	4213	4197	4196.7	33
30	5	Batch 2	6	6650	20	On	4465	4496	4463	4474.7	33
31	5	Batch 2	14	6650	5	On	4653	4685	4665	4667.7	32
32	3	Batch 2	14	6650	5	Off	4683	4712	4677	4690.7	35

(d) Do any of the process variables affect the variability in camber measurements?
(e) If it is important to reduce camber as much as possible, what recommendations would you make?

8-25. A spin coater is used to apply photoresist to a bare silicon wafer. This operation usually occurs early in the semiconductor manufacturing process, and the average coating thickness and the variability in the coating thickness has an important impact on downstream manufacturing steps. Six variables are used in the experiment. The variables and their high and low levels are as follows:

Factor	Low Level	High Level
Final spin speed	7350 rpm	6650 rpm
Acceleration rate	5	20
Volume of resist applied	3 cc	5 cc
Time of spin	14 s	6 s
Resist batch variation	Batch 1	Batch 2
Exhaust pressure	Cover off	Cover on

The experimenter decides to use a 2^{6-1} design and to make three readings on resist thickness on each test wafer. The data are shown in Table 8-30.
(a) Verify that this is a 2^{6-1} design. Discuss the alias relationships in this design.
(b) What factors appear to affect average resist thickness?
(c) Because the volume of resist applied has little effect on average thickness, does this have any important practical implications for the process engineers?
(d) Project this design into a smaller design involving only the significant factors. Graphically display the results. Does this aid in interpretation?
(e) Use the range of resist thickness as a response variable. Is there any indication that any of these factors affect the variability in resist thickness?
(f) Where would you recommend that the process engineers run the process?

8-26. Harry and Judy Peterson-Nedry (two friends of the author) own a vineyard and winery in Newberg, Oregon. They grow several varieties of grapes and manufacture wine. Harry and Judy have used factorial designs for process and product development in the wine-making segment of their business. This problem describes the experiment conducted for their 1985 Pinot Noir. Eight variables, shown below, were originally studied in this experiment:

Variable	Low Level (−)	High Level (+)
A = Pinot Noir clone	Pommard	Wadenswil
B = Oak type	Allier	Troncais
C = Age of barrel	Old	New
D = Yeast/skin contact	Champagne	Montrachet
E = Stems	None	All
F = Barrel toast	Light	Medium
G = Whole cluster	None	10%
H = Fermentation temperature	Low (75°F max)	High (92°F max)

Harry and Judy decided to use a 2_{IV}^{8-4} design with 16 runs. The wine was taste-tested by a panel of experts on March 8, 1986. Each expert ranked the 16 samples of wine tasted, with rank 1 being the best. The design and the taste-test panel results are shown in Table 8-31 on page 356.
(a) What are the alias relationships in the design selected by Harry and Judy?
(b) Use the average ranks ($\bar{y}$) as a response variable. Analyze the data and draw con-

Table 8-31 Design and Results for Wine Tasting Experiment

	Variable								Panel Rankings					Summary	
Run	*A*	*B*	*C*	*D*	*E*	*F*	*G*	*H*	HPN	JPN	CAL	DCM	RGB	$\bar{y}$	*s*
1	−	−	−	−	−	−	−	−	12	6	13	10	7	9.6	3.05
2	+	−	−	−	−	+	+	+	10	7	14	14	9	10.8	3.11
3	−	+	−	−	+	−	+	+	14	13	10	11	15	12.6	2.07
4	+	+	−	−	+	+	−	−	9	9	7	9	12	9.2	1.79
5	−	−	+	−	+	+	+	−	8	8	11	8	10	9.0	1.41
6	+	−	+	−	+	−	−	+	16	12	15	16	16	15.0	1.73
7	−	+	+	−	−	+	−	+	6	5	6	5	3	5.0	1.22
8	+	+	+	−	−	−	+	−	15	16	16	15	14	15.2	0.84
9	−	−	−	+	+	+	−	+	1	2	3	3	2	2.2	0.84
10	+	−	−	+	+	−	+	−	7	11	4	7	6	7.0	2.55
11	−	+	−	+	−	+	+	−	13	3	8	12	8	8.8	3.96
12	+	+	−	+	−	−	−	+	3	1	5	1	4	2.8	1.79
13	−	−	+	+	−	−	+	+	2	10	2	4	5	4.6	3.29
14	+	−	+	+	−	+	−	−	4	4	1	2	1	2.4	1.52
15	−	+	+	+	+	−	−	−	5	15	9	6	11	9.2	4.02
16	+	+	+	+	+	+	+	+	11	14	12	13	13	12.6	1.14

clusions. You will find it helpful to examine a normal probability plot of the effect estimates.

(c) Use the standard deviation of the ranks (or some appropriate transformation such as $\log s$) as a response variable. What conclusions can you draw about the effects of the eight variables on variability in wine quality?

(d) After looking at the results, Harry and Judy decide that one of the panel members (DCM) knows more about beer than he does about wine, so they decide to delete his ranking. What affect would this have on the results and conclusions from parts (b) and (c)?

(e) Suppose that just before the start of the experiment, Harry and Judy discovered that the eight new barrels they ordered from France for use in the experiment would not arrive in time, and all 16 runs would have to be made with old barrels. If Harry and Judy just drop column C from their design, what does this do to the alias relationships? Do they need to start over and construct a new design?

(f) Harry and Judy know from experience that some treatment combinations are unlikely to produce good results. For example, the run with all eight variables at the high level generally results in a poorly rated wine. This was confirmed in the March 8, 1986 taste test. They want to set up a new design for their 1986 Pinot Noir using these same eight variables, but they do not want to make the run with all eight factors at the high level. What design would you suggest?

8-27. In an article in *Quality Engineering* ("An Application of Fractional Factorial Experimental Designs," 1988, Vol. 1, pp. 19–23) M. B. Kilgo describes an experiment to determine the effect of CO_2 pressure (A), CO_2 temperature (B), peanut moisture (C), CO_2 flow rate (D), and peanut particle size (E) on the total yield of oil per batch of peanuts (y). The levels that she used for these factors are as follows:

Coded Level	A, Pressure (bar)	B, Temp. (°C)	C, Moisture (% by weight)	D, Flow (liters/min)	E, Part. Size (mm)
−1	415	25	5	40	1.28
1	550	95	15	60	4.05

She conducted the 16-run fractional factorial experiment shown below.

A	B	C	D	E	y
415	25	5	40	1.28	63
550	25	5	40	4.05	21
415	95	5	40	4.05	36
550	95	5	40	1.28	99
415	25	15	40	4.05	24
550	25	15	40	1.28	66
415	95	15	40	1.28	71
550	95	15	40	4.05	54
415	25	5	60	4.05	23
550	25	5	60	1.28	74
415	95	5	60	1.28	80
550	95	5	60	4.05	33
415	25	15	60	1.28	63
550	25	15	60	4.05	21
415	95	15	60	4.05	44
550	95	15	60	1.28	96

(a) What type of design has been used? Identify the defining relation and the alias relationships.
(b) Estimate the factor effects and use a normal probability plot to tentatively identify the important factors.
(c) Perform an appropriate statistical analysis to test the hypotheses that the factors identified in part (b) above have a significant effect on the yield of peanut oil.
(d) Fit a model that could be used to predict peanut oil yield in terms of the factors that you have identified as important.
(e) Analyze the residuals from this experiment and comment on model adequacy.

8-28. A 16-run fractional factorial experiment in 10 factors on sand-casting of engine manifolds was conducted by engineers at the Essex Aluminum Plant of the Ford Motor Company and described in the article "Evaporative Cast Process 3.0 Liter Intake Manifold Poor Sandfill Study," by D. Becknell (*Fourth Symposium on Taguchi Methods*, American Supplier Institute, Dearborn, MI, 1986, pp. 120–130). The purpose was to determine which of 10 factors has an effect on the proportion of defective castings. The design and the resulting proportion of nondefective castings $\hat{p}$ observed on each run are shown below. This is a resolution III fraction with generators $E = CD$, $F = BD$, $G = BC$, $H = AC$, $J = AB$, and $K = ABC$. Assume that the number of castings made at each run in the design is 1000.

Run	A	B	C	D	E	F	G	H	J	K	$\hat{p}$	$\arcsin\sqrt{\hat{p}}$	F&T's Modification
1	−	−	−	−	+	+	+	+	+	−	0.958	1.364	1.363
2	+	−	−	−	+	+	+	−	−	+	1.000	1.571	1.555
3	−	+	−	−	+	−	−	+	−	+	0.977	1.419	1.417
4	+	+	−	−	+	−	−	−	+	−	0.775	1.077	1.076
5	−	−	+	−	−	+	−	−	+	+	0.958	1.364	1.363
6	+	−	+	−	−	+	−	+	−	−	0.958	1.364	1.363
7	−	+	+	−	−	−	+	−	−	−	0.813	1.124	1.123
8	+	+	+	−	−	−	+	+	+	+	0.906	1.259	1.259
9	−	−	−	+	−	−	+	+	+	−	0.679	0.969	0.968
10	+	−	−	+	−	−	+	−	−	+	0.781	1.081	1.083
11	−	+	−	+	−	+	−	+	−	+	1.000	1.571	1.556
12	+	+	−	+	−	+	−	−	+	−	0.896	1.241	1.242
13	−	−	+	+	+	−	−	−	+	+	0.958	1.364	1.363
14	+	−	+	+	+	−	−	+	−	−	0.818	1.130	1.130
15	−	+	+	+	+	+	+	−	−	−	0.841	1.161	1.160
16	+	+	+	+	+	+	+	+	+	+	0.955	1.357	1.356

(a) Find the defining relation and the alias relationships in this design.
(b) Estimate the factor effects and use a normal probability plot to tentatively identify the important factors.
(c) Fit an appropriate model using the factors identified in part (b) above.
(d) Plot the residuals from this model versus the predicted proportion of nondefective castings. Also prepare a normal probability plot of the residuals. Comment on the adequacy of these plots.
(e) In part (d) you should have noticed an indication that the variance of the response is not constant (considering that the response is a proportion, you should have expected this). The previous table also shows a transformation on $\hat{p}$, the arcsin square

root, that is a widely used *variance stabilizing transformation* for proportion data (refer to the discussion of variance stabilizing transformations in Chapter 3). Repeat parts (a) through (d) above using the transformed response and comment on your results. Specifically, are the residual plots improved?

(f) There is a modification to the arcsin square root transformation, proposed by Freeman and Tukey ("Transformations Related to the Angular and the Square Root," *Annals of Mathematical Statistics*, Vol. 21, 1950, pp. 607–611) that improves its performance in the tails. F&T's modification is:

$$[\arcsin\sqrt{n\hat{p}/(n+1)} + \arcsin\sqrt{(n\hat{p}+1)/(n+1)}]/2$$

Rework parts (a) through (d) using this transformation and comment on the results. (For an interesting discussion and analysis of this experiment, refer to "Analysis of Factorial Experiments with Defects or Defectives as the Response," by S. Bisgaard and H. T. Fuller, *Quality Engineering*, Vol. 7, 1994–95, pp. 429–443.)

8-29. A 16-run fractional factorial experiment in nine factors was conducted by Chrysler Motors Engineering and described in the article "Sheet Molded Compound Process Improvement," by P. I. Hsieh and D. E. Goodwin (*Fourth Symposium on Taguchi Methods*, American Supplier Institute, Dearborn, MI, 1986, pp. 13–21). The purpose was to reduce the number of defects in the finish of sheet-molded grill opening panels. The design, and the resulting number of defects, c, observed on each run, is shown below. This is a resolution III fraction with generators $E = BD$, $F = BCD$, $G = AC$, $H = ACD$, and $J = AB$.

Run	A	B	C	D	E	F	G	H	J	c	$\sqrt{c}$	F&T's Modification
1	−	−	−	−	+	−	+	−	+	56	7.48	7.52
2	+	−	−	−	+	−	−	+	−	17	4.12	4.18
3	−	+	−	−	−	+	+	−	−	2	1.41	1.57
4	+	+	−	−	−	+	−	+	+	4	2.00	2.12
5	−	−	+	−	+	+	−	+	+	3	1.73	1.87
6	+	−	+	−	+	+	+	−	−	4	2.00	2.12
7	−	+	+	−	−	−	−	+	−	50	7.07	7.12
8	+	+	+	−	−	−	+	−	+	2	1.41	1.57
9	−	−	−	+	−	+	+	+	+	1	1.00	1.21
10	+	−	−	+	−	+	−	−	−	0	0.00	0.50
11	−	+	−	+	+	−	+	+	−	3	1.73	1.87
12	+	+	−	+	+	−	−	−	+	12	3.46	3.54
13	−	−	+	+	−	−	−	−	+	3	1.73	1.87
14	+	−	+	+	−	−	+	+	−	4	2.00	2.12
15	−	+	+	+	+	+	−	−	−	0	0.00	0.50
16	+	+	+	+	+	+	+	+	+	0	0.00	0.50

(a) Find the defining relation and the alias relationships in this design.

(b) Estimate the factor effects and use a normal probability plot to tentatively identify the important factors.

(c) Fit an appropriate model using the factors identified in part (b) above.

(d) Plot the residuals from this model versus the predicted number of defects. Also, prepare a normal probability plot of the residuals. Comment on the adequacy of these plots.

(e) In part (d) you should have noticed an indication that the variance of the response is not constant (considering that the response is a count, you should have expected this). The previous table also shows a transformation on c, the square root, that is a widely used *variance stabilizing transformation* for count data (refer to the discussion of variance stabilizing transformations in Chapter 3). Repeat parts (a) through (d) using the transformed response and comment on your results. Specifically, are the residual plots improved?

(f) There is a modification to the square root transformation, proposed by Freeman and Tukey ("Transformations Related to the Angular and the Square Root," *Annals of Mathematical Statistics*, Vol. 21, 1950, pp. 607–611) that improves its performance. F&T's modification to the square root transformation is

$$[\sqrt{c} + \sqrt{(c + 1)}]/2$$

Rework parts (a) through (d) using this transformation and comment on the results. (For an interesting discussion and analysis of this experiment, refer to "Analysis of Factorial Experiments with Defects or Defectives as the Response," by S. Bisgaard and H. T. Fuller, *Quality Engineering*, Vol. 7, 1994–1995, pp. 429–443.)

8-30. An experiment is run in a semiconductor factory to investigate the effect of six factors on transistor gain. The design selected is the 2^{6-2}_{IV} shown below:

Standard Order	Run Order	A	B	C	D	E	F	Gain
1	2	−	−	−	−	−	−	1455
2	8	+	−	−	−	+	−	1511
3	5	−	+	−	−	+	+	1487
4	9	+	+	−	−	−	+	1596
5	3	−	−	+	−	+	+	1430
6	14	+	−	+	−	−	+	1481
7	11	−	+	+	−	−	−	1458
8	10	+	+	+	−	+	−	1549
9	15	−	−	−	+	−	+	1454
10	13	+	−	−	+	+	+	1517
11	1	−	+	−	+	+	−	1487
12	6	+	+	−	+	−	−	1596
13	12	−	−	+	+	+	−	1446
14	4	+	−	+	+	−	−	1473
15	7	−	+	+	+	−	+	1461
16	16	+	+	+	+	+	+	1563

(a) Use a normal plot of the effects to identify the significant factors.

(b) Conduct appropriate statistical tests for the model identified in part (a).

(c) Analyze the residuals and comment on your findings.

(d) Can you find a set of operating conditions that produce gain of 1500 ± 25?

8-31. Heat treating is often used to carbonize metal parts, such as gears. The thickness of the carbonized layer is a critical output variable from this process, and it is usually measured by performing a carbon analysis on the gear pitch (the top of the gear tooth). Six factors were studied in a 2^{6-2}_{IV} design: A = furnace temperature, B = cycle time, C = carbon

concentration, D = duration of the carbonizing cycle, E = carbon concentration of the diffuse cycle, and F = duration of the diffuse cycle. The experiment is shown below:

Standard Order	Run Order	A	B	C	D	E	F	Pitch
1	5	−	−	−	−	−	−	74
2	7	+	−	−	−	+	−	190
3	8	−	+	−	−	+	+	133
4	2	+	+	−	−	−	+	127
5	10	−	−	+	−	+	+	115
6	12	+	−	+	−	−	+	101
7	16	−	+	+	−	−	−	54
8	1	+	+	+	−	+	−	144
9	6	−	−	−	+	−	+	121
10	9	+	−	−	+	+	+	188
11	14	−	+	−	+	+	−	135
12	13	+	+	−	+	−	−	170
13	11	−	−	+	+	+	−	126
14	3	+	−	+	+	−	−	175
15	15	−	+	+	+	−	+	126
16	4	+	+	+	+	+	+	193

(a) Estimate the factor effects and plot them on a normal probability plot. Select a tentative model.
(b) Perform appropriate statistical tests on the model.
(c) Analyze the residuals and comment on model adequacy.
(d) Interpret the results of this experiment. Assume that a layer thickness of between 140 and 160 is desirable.

8-32. Five factors are studied in the irregular fractional factorial design of resolution V shown below:

Standard Order	Run Order	A	B	C	D	E	y
1	1	−	−	−	−	−	16.33
2	10	−	+	−	−	−	18.43
3	5	+	+	−	−	−	27.07
4	4	−	−	+	−	−	16.95
5	15	+	−	+	−	−	14.58
6	19	−	+	+	−	−	19.12
7	16	−	−	−	+	−	18.96
8	7	+	−	−	+	−	23.56
9	8	+	+	−	+	−	29.15
10	3	+	−	+	+	−	15.74
11	13	−	+	+	+	−	20.73
12	11	+	+	+	+	−	21.52
13	12	−	−	−	−	+	15.58
14	20	+	−	−	−	+	21.03
15	9	+	+	−	−	+	26.78

Standard Order	Run Order	A	B	C	D	E	y
16	22	+	−	+	−	+	13.39
17	21	−	+	+	−	+	18.63
18	6	+	+	+	−	+	19.01
19	23	−	−	−	+	+	17.96
20	18	−	+	−	+	+	20.49
21	24	+	+	−	+	+	29.31
22	17	−	−	+	+	+	17.62
23	2	+	−	+	+	+	16.03
24	14	−	+	+	+	+	21.42

(a) Analyze the data from this experiment. What factors influence the response y?
(b) Analyze the residuals. Comment on model adequacy.

9 Three-Level and Mixed-Level Factorial and Fractional Factorial Designs

The two-level series of factorial and fractional factorial designs discussed in Chapters 6, 7, and 8 are widely used in industrial research and development. There are some extensions and variations of these designs that are occasionally useful, such as the designs for cases where all the factors are present at three levels. These 3^k designs will be discussed in this chapter. We will also consider cases where some factors have two levels and other factors have either three or four levels.

9-1 THE 3^k FACTORIAL DESIGN

9-1.1 Notation and Motivation for the 3^k Design

We now discuss the 3^k factorial design; that is, a factorial arrangement with k factors each at three levels. Factors and interactions will be denoted by capital letters. We will refer to the three levels of the factors as low, intermediate, and high. There are several different notations used to represent these factor levels; one possibility is to represent the factor levels by the digits 0 (low), 1 (intermediate), and 2 (high). Each treatment combination in the 3^k design will be denoted by k digits, where the first digit indicates the level of factor A, the second digit indicates the level of factor $B, \ldots,$ and the kth digit indicates the level of factor K. For example, in a 3^2 design, 00 denotes the treatment combination corresponding to A and B both at the low level, and 01 denotes the treatment combination corresponding to A at the low level and B at the intermediate level. Figures 9-1 and 9-2 (on the next page) show the geometry of the 3^2 and the 3^3 design, respectively, using this notation.

This system of notation could have been used for the 2^k designs presented previously, with 0 and 1 used in place of the minus and plus 1s, respectively. In the 2^k design, we prefer the ± 1 notation because it facilitates the geometric view of the design and because it is directly applicable to regression modeling, blocking, and the construction of fractional factorials.

In the 3^k system of designs, when the factors are **quantitative**, we often denote the low, intermediate, and high levels by -1, 0, and $+1$, respectively. This facilitates fitting

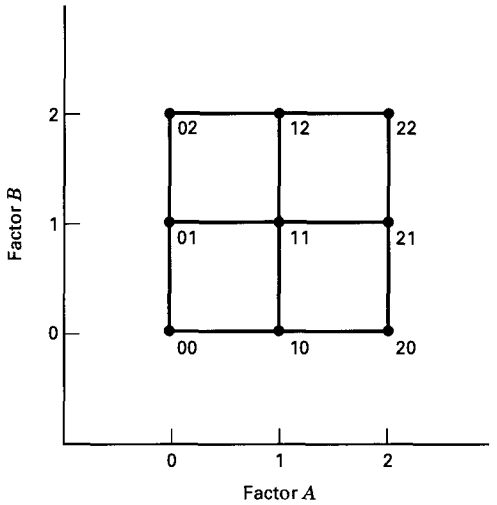


Figure 9-1 Treatment combinations in a 3^2 design.

a **regression model** relating the response to the factor levels. For example, consider the 3^2 design in Figure 9-1, and let x_1 represent factor A and x_2 represent factor B. A regression model relating the response y to x_1 and x_2 that is supported by this design is

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \epsilon \qquad (9\text{-}1)$$

Notice that the addition of a third factor level allows the relationship between the response and the design factors to be modeled as a quadratic.

The 3^k design is certainly a possible choice by an experimenter who is concerned about curvature in the response function. However, two points need to be considered:

1. The 3^k design is not the most efficient way to model a quadratic relationship; the **response surface designs** discussed in Chapter 11 are superior alternatives.

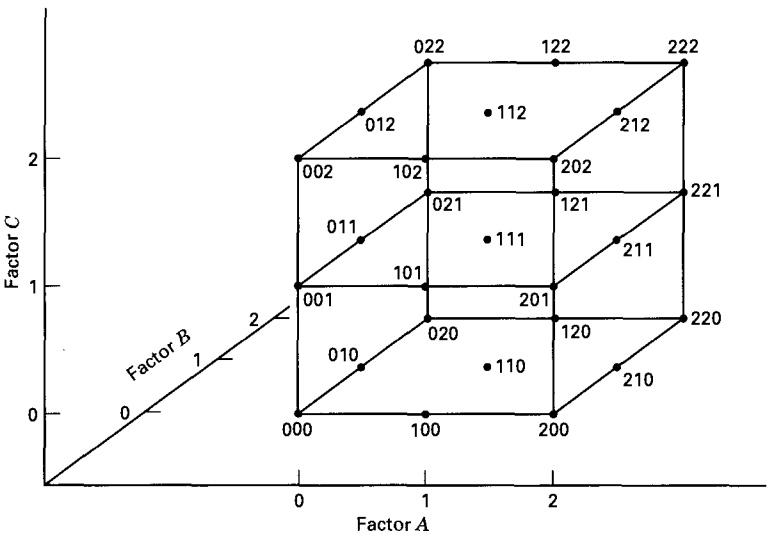


Figure 9-2 Treatment combinations in a 3^3 design.

2. The 2^k design augmented with center points, as discussed in Chapter 6, is an excellent way to obtain an indication of curvature. It allows one to keep the size and complexity of the design low and simultaneously obtain some protection against curvature. Then, if curvature is important, the two-level design can be augmented with **axial runs** to obtain a **central composite design**, as shown in Figure 6-36. This **sequential strategy** of experimentation is far more efficient than running a 3^k factorial design with quantitative factors.

9-1.2 The 3^2 Design

The simplest design in the 3^k system is the 3^2 design, which has two factors, each at three levels. The treatment combinations for this design were shown in Figure 9-1. Because there are $3^2 = 9$ treatment combinations, there are eight degrees of freedom between these treatment combinations. The main effects of A and B each have two degrees of freedom, and the AB interaction has four degrees of freedom. If there are n replicates, there will be $n3^2 - 1$ total degrees of freedom and $3^2(n - 1)$ degrees of freedom for error.

The sums of squares for A, B, and AB may be computed by the usual methods for factorial designs discussed in Chapter 5. Each main effect can be represented by a linear and a quadratic component, each with a single degree of freedom, as demonstrated in Equation 9-1. Of course, this is only meaningful if the factor is quantitative.

The two-factor interaction AB may be partitioned in two ways. The first method consists of subdividing AB into the four single-degree-of-freedom components corresponding to $AB_{L\times L}$, $AB_{L\times Q}$, $AB_{Q\times L}$, and $AB_{Q\times Q}$. This can be done by fitting the terms $\beta_{12}x_1x_2$, $\beta_{122}x_1x_2^2$, $\beta_{112}x_1^2x_2$, and $\beta_{1122}x_1^2x_2^2$, respectively, as demonstrated in Example 5-5. For the tool life data, this yields $SS_{AB_{L\times L}} = 8.00$, $SS_{AB_{L\times Q}} = 42.67$, $SS_{AB_{Q\times L}} = 2.67$, and $SS_{AB_{Q\times Q}} = 8.00$. Because this is an orthogonal partitioning of AB, note that $SS_{AB} = SS_{AB_{L\times L}} + SS_{AB_{L\times Q}} + SS_{AB_{Q\times L}} + SS_{AB_{Q\times Q}} = 61.34$.

The second method is based on **orthogonal Latin squares**. Consider the totals of the treatment combinations for the data in Example 5-5. These totals are shown in Figure 9-3 as the circled numbers in the squares. The two factors A and B correspond to the rows and columns, respectively, of a 3×3 Latin square. In Figure 9-3, two particular 3×3 Latin squares are shown superimposed on the cell totals.

These two Latin squares are **orthogonal**; that is, if one square is superimposed on

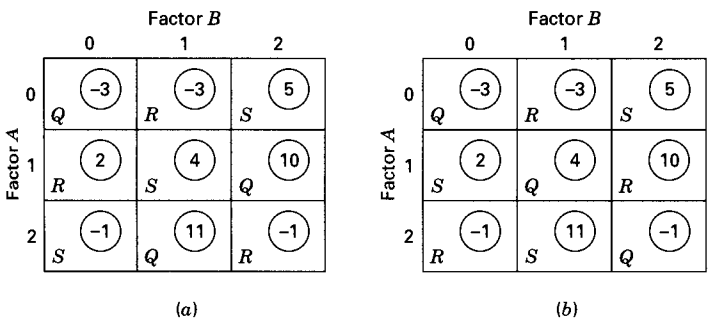


Figure 9-3 Treatment combination totals from Example 5-5 with two orthogonal Latin squares superimposed.

the other, each letter in the first square will appear exactly once with each letter in the second square. The totals for the letters in the (*a*) square are $Q = 18$, $R = -2$, and $S = 8$, and the sum of squares between these totals is $[18^2 + (-2)^2 + 8^2]/(3)(2) - [24^2/(9)(2)] = 33.34$, with two degrees of freedom. Similarly, the letter totals in the (*b*) square are $Q = 0$, $R = 6$, and $S = 18$, and the sum of squares between these totals is $[0^2 + 6^2 + 18^2]/(3)(2) - [24^2/(9)(2)] = 28.00$, with two degrees of freedom. Note that the sum of these two components is

$$33.34 + 28.00 = 61.34 = SS_{AB}$$

with $2 + 2 = 4$ degrees of freedom.

In general, the sum of squares computed from square (*a*) is called the ***AB* component of interaction**, and the sum of squares computed from square (*b*) is called ***AB*^{2} component of interaction**. The components AB and AB^2 each have two degrees of freedom. This terminology is used because if we denote the levels (0, 1, 2) for A and B by x_1 and x_2, respectively, then we find that the letters occupy cells according to the following pattern:

Square (*a*)	Square (*b*)
Q: $x_1 + x_2 = 0 \pmod 3$	Q: $x_1 + 2x_2 = 0 \pmod 3$
R: $x_1 + x_2 = 1 \pmod 3$	S: $x_1 + 2x_2 = 1 \pmod 3$
S: $x_1 + x_2 = 2 \pmod 3$	R: $x_1 + 2x_2 = 2 \pmod 3$

For example, in square (*b*), note that the middle cell corresponds to $x_1 = 1$ and $x_2 = 1$; thus, $x_1 + 2x_2 = 1 + (2)(1) = 3 = 0 \pmod 3$, and Q would occupy the middle cell. When considering expressions of the form A^pB^q, we establish the convention that the only exponent allowed on the first letter is 1. If the first letter exponent is not 1, the entire expression is squared and the exponents are reduced modulus 3. For example, A^2B is the same as AB^2 because

$$A^2B = (A^2B)^2 = A^4B^2 = AB^2$$

The AB and AB^2 components of the AB interaction have no actual meaning and are usually not displayed in the analysis of variance table. However, this rather arbitrary partitioning of the AB interaction into two orthogonal two-degree-of-freedom components is very useful in constructing more complex designs. Also, there is no connection between the AB and AB^2 components of interaction and the sums of squares for $AB_{L\times L}$, $AB_{L\times Q}$, $AB_{Q\times L}$, and $AB_{Q\times Q}$.

The AB and AB^2 components of interaction may be computed another way. Consider the treatment combination totals in either square in Figure 9-3. If we add the data by diagonals downward from left to right, we obtain the totals $-3 + 4 - 1 = 0$, $-3 + 10 - 1 = 6$, and $5 + 11 + 2 = 18$. The sum of squares between these totals is 28.00 (AB^2). Similarly, the diagonal totals downward from right to left are $5 + 4 - 1 = 8$, $-3 + 2 - 1 = -2$, and $-3 + 11 + 10 = 18$. The sum of squares between these totals is 33.34 (AB). Yates called these components of interaction the ***I* and *J* components of interaction**, respectively. We use both notations interchangeably; that is,

$$I(AB) = AB^2$$
$$J(AB) = AB$$

9-1.3 The 3^3 Design

Now suppose there are three factors (A, B, and C) under study, and each factor is at three levels arranged in a factorial experiment. This is a 3^3 factorial design, and the experimental layout and treatment combination notation were shown previously in Figure 9-2. The 27 treatment combinations have 26 degrees of freedom. Each main effect has 2 degrees of freedom, each two-factor interaction has 4 degrees of freedom, and the three-factor interaction has 8 degrees of freedom. If there are n replicates, there are $n3^3 - 1$ total degrees of freedom and $3^3(n - 1)$ degrees of freedom for error.

The sums of squares may be calculated using the standard methods for factorial designs. In addition, if the factors are quantitative the main effects may be partitioned into linear and quadratic components, each with a single degree of freedom. The two-factor interactions may be decomposed into linear $\times$ linear, linear $\times$ quadratic, quadratic $\times$ linear, and quadratic $\times$ quadratic effects. Finally, the three-factor interaction ABC can be partitioned into eight single-degree-of-freedom components corresponding to linear $\times$ linear $\times$ linear, linear $\times$ linear $\times$ quadratic, and so on. Such a breakdown for the three-factor interaction is generally not very useful.

It is also possible to partition the two-factor interactions into their I and J components. These would be designated AB, AB^2, AC, AC^2, BC, and BC^2, and each component would have two degrees of freedom. As in the 3^2 design, these components have no physical significance.

The three-factor interaction ABC may be partitioned into four orthogonal two-degrees-of-freedom components, which are usually called the W, X, Y, and Z components of the interaction. They are also referred to as the AB^2C^2, AB^2C, ABC^2, and ABC components of the ABC interaction, respectively. The two notations are used interchangeably; that is,

$$\begin{aligned} W(ABC) &= AB^2C^2 \\ X(ABC) &= AB^2C \\ Y(ABC) &= ABC^2 \\ Z(ABC) &= ABC \end{aligned}$$

Note that no first letter can have an exponent other than 1. Like the I and J components, the W, X, Y, and Z components have no practical interpretation. They are, however, useful in constructing more complex designs.

EXAMPLE 9-1

A machine is used to fill 5-gallon metal containers with soft drink syrup. The variable of interest is the amount of syrup loss due to frothing. Three factors are thought to influence frothing: the nozzle design (A), the filling speed (B), and the operating pressure (C). Three nozzles, three filling speeds, and three pressures are chosen and two replicates of a 3^3 factorial experiment are run. The coded data are shown in Table 9-1 on page 368.

The analysis of variance for the syrup loss data is shown in Table 9-2 on page 368. The sums of squares have been computed by the usual methods. We see that the filling speed and operating pressure are statistically significant. All three two-factor interactions are also significant. The two-factor interactions are analyzed graphically in Figure 9-4 on page 369. The middle level of speed gives the best performance, nozzle types 2 and 3, and either the low (10 psi) or high (20 psi) pressure seem most effective in reducing syrup loss.

Table 9-1 Syrup Loss Data for Example 9-1 (units are cubic centimeters − 70)

	Nozzle Type (A)								
	1			2			3		
Pressure (in psi)	Speed (in RPM) (B)								
(C)	100	120	140	100	120	140	100	120	140
10	−35	−45	−40	17	−65	20	−39	−55	15
	−25	−60	15	24	−58	4	−35	−67	−30
15	110	−10	80	55	−55	110	90	−28	110
	75	30	54	120	−44	44	113	−26	135
20	4	−40	31	−23	−64	−20	−30	−61	54
	5	−30	36	−5	−62	−31	−55	−52	4

Example 9-1 illustrates a situation where the three-level design often finds some application; one or more of the factors is **qualitative**, naturally taking on three levels, and the remaining factors are **quantitative**. In this example, suppose that there are only three nozzle designs that are of interest. This is clearly, then, a qualitative factor that requires three levels. The filling speed and the operating pressure are quantitative factors. Therefore, we could fit a quadratic model such as Equation 9-1 in the two factors speed and pressure at each level of the nozzle factor.

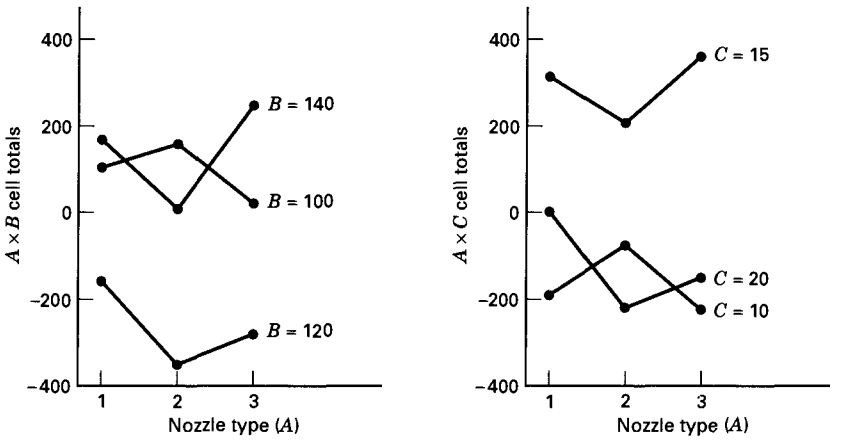
Table 9-3 (on the facing page) shows these quadratic regression models. The β's in these models were estimated using a standard linear regression computer program. (We will discuss least squares regression in more detail in Chapter 10.) In these models, the variables x_1 and x_2 are coded to the levels -1, 0, $+1$ as discussed previously, and we assumed the following natural levels for pressure and speed:

Coded Level	Speed (psi)	Pressure (rpm)
−1	100	10
0	120	15
+1	140	20

Table 9-3 presents models both in terms of these coded variables and in terms of the natural levels of speed and pressure.

Table 9-2 Analysis of Variance for Syrup Loss Data

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
A, nozzle	993.77	2	496.89	1.17	0.3256
B, speed	61,190.33	2	30,595.17	71.74	<0.0001
C, pressure	69,105.33	2	34,552.67	81.01	<0.0001
AB	6,300.90	4	1,575.22	3.69	0.0383
AC	7,513.90	4	1,878.47	4.40	0.0222
BC	12,854.34	4	3,213.58	7.53	0.0025
ABC	4,628.76	8	578.60	1.36	0.2737
Error	11,515.50	27	426.50		
Total	174,102.83	53			



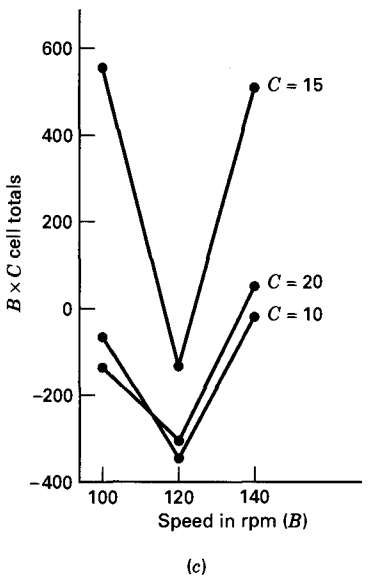


Figure 9-4 Two-factor interactions for Example 9-1.

Table 9-3 Regression Models for Example 9-1

Nozzle Type	x_1 = Speed (S), x_2 = Pressure (P) in Coded Units
1	$\hat{y} = 22.1 + 3.5x_1 + 16.3x_2 + 51.7x_1^2 - 71.8x_2^2 + 2.9x_1x_2$
	$\hat{y} = 1217.3 - 31.256S + 86.017P + 0.12917S^2 - 2.8733P^2 + 0.02875SP$
2	$\hat{y} = 25.6 - 22.8x_1 - 12.3x_2 + 14.1x_1^2 - 56.9x_2^2 - 0.7x_1x_2$
	$\hat{y} = 180.1 - 9.475S + 66.75P + 0.035S^2 - 2.2767P^2 - 0.0075SP$
3	$\hat{y} = 15.1 + 20.3x_1 + 5.9x_2 + 75.8x_1^2 - 94.9x_2^2 + 10.5x_1x_2$
	$\hat{y} = 1940.1 - 40.058S + 102.48P + 0.18958S^2 - 3.7967P^2 + 0.105SP$

Figure 9-5 shows the response surface contour plots of constant syrup loss as a function of speed and pressure for each nozzle type. These plots reveal considerable useful information about the performance of this filling system. Because the objective is to minimize syrup loss, nozzle type 3 would be preferred as the smallest observed contours (-60) appear only on this plot. Filling speed near the middle level of 120 rpm and either the low or high pressure levels should be used.

When constructing contour plots for an experiment that has a mixture of quantitative and qualitative factors, it is not unusual to find that the shapes of the surfaces in the quantitative factors are very different at each level of the qualitative factors. This is noticeable to some degree in Figure 9-5, where the shape of the surface for nozzle type 2 is considerably elongated in comparison to the surfaces for nozzle types 1 and 3. When this occurs, it implies that the optimum operating conditions (and other important conclusions) in terms of the quantitative factors are very different at each level of the qualitative factors.

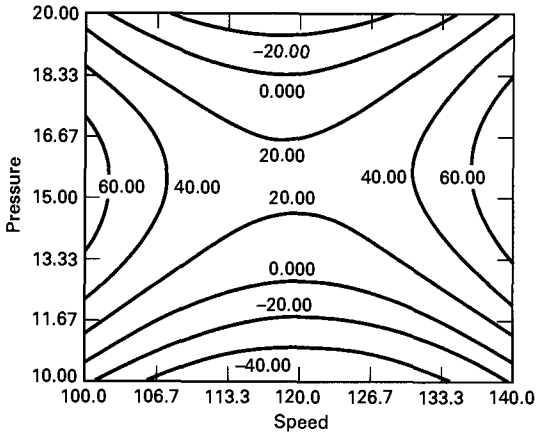
We can easily show the numerical partitioning of the ABC interaction into its four orthogonal two-degree-of-freedom components using the data in Example 9-1. The general procedure has been described by Cochran and Cox (1957) and Davies (1956). First, select any two of the three factors, say AB, and compute the I and J totals of the AB interaction at each level of the third factor C. These calculations follow:

		A			Totals	
C	B	1	2	3	I	J
	100	−60	41	−74	−198	−222
10	120	−105	−123	−122	−106	−79
	140	−25	24	−15	−155	−158
	100	185	175	203	331	238
15	120	20	−99	−54	255	440
	140	134	154	245	377	285
	100	9	−28	−85	−59	−144
20	120	−70	−126	−113	−74	−40
	140	67	−51	58	−206	−155

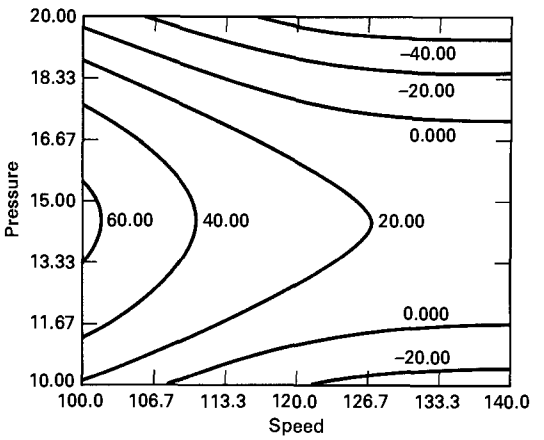
The $I(AB)$ and $J(AB)$ totals are now arranged in a two-way table with factor C, and the I and J diagonal totals of this new display are computed:

				Totals						Totals	
C		$I(AB)$		I	J	C		$J(AB)$		I	J
10	−198	−106	−155	−149	41	10	−222	−79	−158	63	138
15	331	255	377	212	19	15	238	440	285	62	4
20	−59	−74	−206	102	105	20	−144	−40	−155	40	23

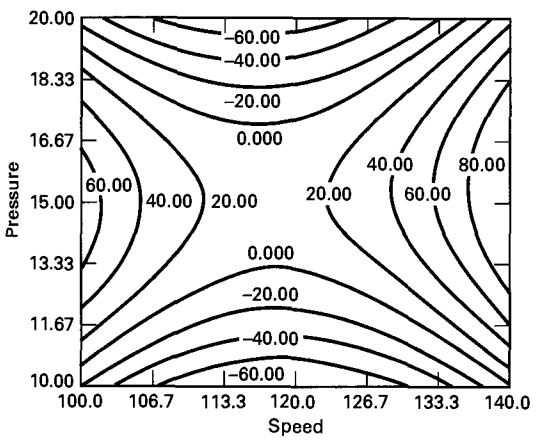
The I and J diagonal totals computed above are actually the totals representing the quantities $I[I(AB) \times C] = AB^2C^2$, $J[I(AB) \times C] = AB^2C$, $I[J(AB) \times C] = ABC^2$, and



(*a*) Nozzle type 1



(*b*) Nozzle type 2



(*c*) Nozzle type 3

Figure 9-5 Contours of constant syrup loss (units: cc − 70) as a function of speed and pressure for nozzle types 1, 2, and 3, Example 9-1.

$J[J(AB) \times C] = ABC$, or the W, X, Y, and Z components of ABC. The sums of squares are found in the usual way; that is,

$$
\begin{aligned}
I[I(AB) \times C)] &= AB^2C^2 = W(ABC) \\
&= \frac{(-149)^2 + (212)^2 + (102)^2}{18} - \frac{(165)^2}{54} = 3804.11 \\
J[I(AB) \times C] &= AB^2C = X(ABC) \\
&= \frac{(41)^2 + (19)^2 + (105)^2}{18} - \frac{(165)^2}{54} = 221.77 \\
I[J(AB) \times C] &= ABC^2 = Y(ABC) \\
&= \frac{(63)^2 + (62)^2 + (40)^2}{18} - \frac{(165)^2}{54} = 18.77 \\
J[J(AB \times C] &= ABC = Z(ABC) \\
&= \frac{(138)^2 + (4)^2 + (23)^2}{18} - \frac{(165)^2}{54} = 584.11
\end{aligned}
$$

Although this is an orthogonal partitioning of SS_{ABC}, we point out again that it is not customarily displayed in the analysis of variance table. In subsequent sections, we discuss the occasional need for the computation of one or more of these components.

9-1.4 The General 3^k Design

The concepts utilized in the 3^2 and 3^3 designs can be readily extended to the case of k factors, each at three levels, that is, to a 3^k factorial design. The usual digital notation is employed for the treatment combinations, so 0120 represents a treatment combination in a 3^4 design with A and D at the low levels, B at the intermediate level, and C at the high level. There are 3^k treatment combinations, with $3^k - 1$ degrees of freedom between them. These treatment combinations allow sums of squares to be determined for k main effects, each with two degrees of freedom; $\binom{k}{2}$ two-factor interactions, each with four degrees of freedom; . . . ; and one k-factor interaction with 2^k degrees of freedom. In general, an h-factor interaction has 2^h degrees of freedom. If there are n replicates, there are $n3^k - 1$ total degrees of freedom and $3^k(n - 1)$ degrees of freedom for error.

Sums of squares for effects and interactions are computed by the usual methods for factorial designs. Typically, three-factor and higher interactions are not broken down any further. However, any h-factor interaction has 2^{h-1} orthogonal two-degrees-of-freedom components. For example, the four-factor interaction $ABCD$ has $2^{4-1} = 8$ orthogonal two-degrees-of-freedom components, denoted by $ABCD^2$, ABC^2D, AB^2CD, $ABCD$, ABC^2D^2, AB^2C^2D, AB^2CD^2, and $AB^2C^2D^2$. In writing these components, note that the only exponent allowed on the first letter is 1. If the exponent on the first letter is not 1, then the entire expression must be squared and the exponents reduced modulus 3. To demonstrate, consider

$$A^2BCD = (A^2BCD)^2 = A^4B^2C^2D^2 = AB^2C^2D^2$$

These interaction components have no physical interpretation, but they are useful in constructing more complex designs.

The size of the design increases rapidly with k. For example, a 3^3 design has 27 treatment combinations per replication, a 3^4 design has 81, a 3^5 design has 243, and so on. Therefore, frequently only a single replicate of the 3^k design is considered, and higher-order interactions are combined to provide an estimate of error. As an illustration, if

three-factor and higher interactions are negligible, then a single replicate of the 3^3 design provides 8 degrees of freedom for error, and a single replicate of the 3^4 design provides 48 degrees of freedom for error. These are still large designs for $k \geq 3$ factors, and, consequently, not too useful.

9-2 CONFOUNDING IN THE 3^k FACTORIAL DESIGN

Even when a single replicate of the 3^k design is considered, the design requires so many runs that it is unlikely that all 3^k runs can be made under uniform conditions. Thus, confounding in blocks is often necessary. The 3^k design may be confounded in 3^p incomplete blocks, where $p < k$. Thus, these designs may be confounded in three blocks, nine blocks, and so on.

9-2.1 The 3^k Factorial Design in Three Blocks

Suppose that we wish to confound the 3^k design in three incomplete blocks. These three blocks have two degrees of freedom among them; thus, there must be two degrees of freedom confounded with blocks. Recall that in the 3^k factorial series each main effect has two degrees of freedom. Furthermore, every two-factor interaction has four degrees of freedom and can be decomposed into two components of interaction (e.g., AB and AB^2), each with two degrees of freedom; every three-factor interaction has eight degrees of freedom and can be decomposed into four components of interaction (e.g., ABC, ABC^2, AB^2C, and AB^2C^2), each with two degrees of freedom; and so on. Therefore, it is convenient to confound a component of interaction with blocks.

The general procedure is to construct a **defining contrast**

$$L = \alpha_1 x_1 + \alpha_2 x_2 + \cdots + \alpha_k x_k \tag{9-2}$$

where α_i represents the exponent on the ith factor in the effect to be confounded and x_i is the level of the ith factor in a particular treatment combination. For the 3^k series, we have $\alpha_i = 0$, 1, or 2 with the first nonzero α_i being unity, and $x_i = 0$ (low level), 1 (intermediate level), or 2 (high level). The treatment combinations in the 3^k design are assigned to blocks based on the value of L (mod 3). Because L (mod 3) can take on only the values 0, 1, or 2, three blocks are uniquely defined. The treatment combinations satisfying $L = 0$ (mod 3) constitute the **principal block**. This block will always contain the treatment combination 00 . . . 0.

For example, suppose we wish to construct a 3^2 factorial design in three blocks. Either component of the AB interaction, AB or AB^2, may be confounded with blocks. Arbitrarily choosing AB^2, we obtain the defining contrast

$$L = x_1 + 2x_2$$

The value of L (mod 3) of each treatment combination may be found as follows:

$$\begin{array}{llll}
00: & L = 1(0) + 2(0) = 0 = 0 \pmod 3 & 11: & L = 1(1) + 2(1) = 3 = 0 \pmod 3 \\
01: & L = 1(0) + 2(1) = 2 = 2 \pmod 3 & 21: & L = 1(2) + 2(1) = 4 = 1 \pmod 3 \\
02: & L = 1(0) + 2(2) = 4 = 1 \pmod 3 & 12: & L = 1(1) + 2(2) = 5 = 2 \pmod 3 \\
10: & L = 1(1) + 2(0) = 1 = 1 \pmod 3 & 22: & L = 1(2) + 2(2) = 6 = 0 \pmod 3
\end{array}$$

$$20: \quad L = 1(2) + 2(0) = 2 = 2 \pmod 3$$

The blocks are shown in Figure 9-6 on the next page.

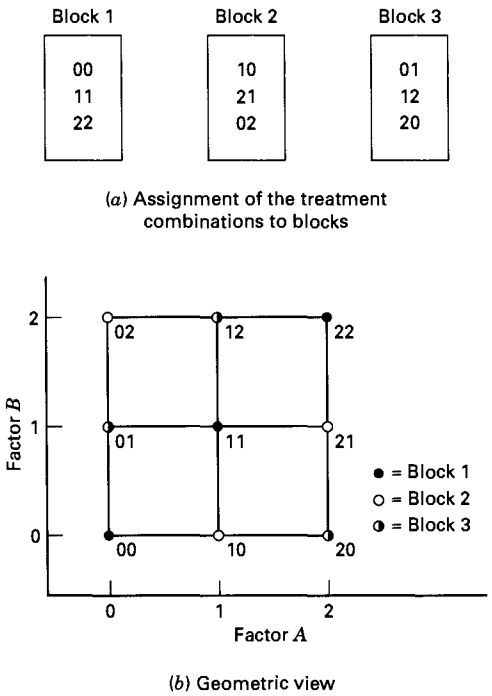


Figure 9-6 The 3^2 design in three blocks with AB^2 confounded.

The elements in the principal block form a group with respect to addition modulus 3. Referring to Figure 9-6, we see that 11 + 11 = 22, and 11 + 22 = 00. Treatment combinations in the other two blocks may be generated by adding, modulus 3, any element in the new block to the elements of the principal block. Thus, for block 2 we use 10 and obtain

$$10 + 00 = 10 \qquad 10 + 11 = 21 \qquad \text{and} \qquad 10 + 22 = 02$$

To generate block 3, using 01 we find

$$01 + 00 = 01 \qquad 01 + 11 = 12 \qquad \text{and} \qquad 01 + 22 = 20$$

EXAMPLE 9-2

We illustrate the statistical analysis of the 3^2 design confounded in three blocks by using the following data, which come from the single replicate of the 3^2 design shown in Figure 9-6.

	Block 1	Block 2	Block 3
	00 = 4	10 = −2	01 = 5
	11 = −4	21 = 1	12 = −5
	22 = 0	02 = 8	20 = 0
Block Totals =	0	7	0

Using conventional methods for the analysis of factorials, we find that $SS_A = 131.56$ and $SS_B = 0.22$.

Table 9-4 Analysis of Variance for Data in Example 9-2

Source of Variation	Sum of Squares	Degrees of Freedom
Blocks (AB^2)	10.89	2
A	131.56	2
B	0.22	2
AB	2.89	2
Total	145.56	8

We also find that

$$SS_{\text{Blocks}} = \frac{(0)^2 + (7)^2 + (0)^2}{3} - \frac{(7)^2}{9} = 10.89$$

However, SS_{Blocks} is exactly equal to the AB^2 component of interaction. To see this, write the observations as follows:

		Factor B		
		0	1	2
Factor A	0	4	5	8
	1	−2	−4	−5
	2	0	1	0

Recall from Section 9-1.2 that the I or AB^2 component of the AB interaction may be found by computing the sum of squares between the left-to-right diagonal totals in the above layout. This yields

$$SS_{AB^2} = \frac{(0)^2 + (0)^2 + (7)^2}{3} - \frac{(7)^2}{9} = 10.89$$

which is identical to SS_{Blocks}.

The analysis of variance is shown in Table 9-4. Because there is only one replicate, no formal tests can be performed. It is not a good idea to use the AB component of interaction as an estimate of error.

We now look at a slightly more complicated design—a 3^3 factorial confounded in three blocks of nine runs each. The AB^2C^2 component of the three-factor interaction will be confounded with blocks. The defining contrast is

$$L = x_1 + 2x_2 + 2x_3$$

It is easy to verify that the treatment combinations 000, 012, and 101 belong in the principal block. The remaining runs in the principal block are generated as follows:

(1) 000 (4) 101 + 101 = 202 (7) 101 + 021 = 122
(2) 012 (5) 012 + 012 = 021 (8) 012 + 202 = 211
(3) 101 (6) 101 + 012 = 110 (9) 021 + 202 = 220

To find the runs in another block, note that the treatment combination 200 is not in the principal block. Thus, the elements of block 2 are

(1) 200 + 000 = 200	(4) 200 + 202 = 102	(7) 200 + 122 = 022
(2) 200 + 012 = 212	(5) 200 + 021 = 221	(8) 200 + 211 = 111
(3) 200 + 101 = 001	(6) 200 + 110 = 010	(9) 200 + 220 = 120

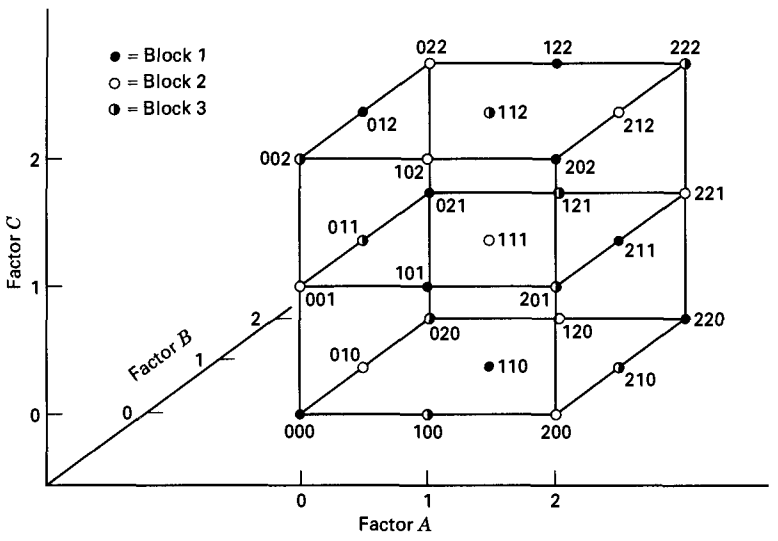
Notice that these runs all satisfy $L = 2 \pmod 3$. The final block is found by observing that 100 does not belong in block 1 or 2. Using 100 as above yields

(1) 100 + 000 = 100	(4) 100 + 202 = 002	(7) 100 + 122 = 222
(2) 100 + 012 = 112	(5) 100 + 021 = 121	(8) 100 + 211 = 011
(3) 100 + 101 = 201	(6) 100 + 110 = 210	(9) 100 + 220 = 020

The blocks are shown in Figure 9-7.

Block 1	Block 2	Block 3
000	200	100
012	212	112
101	001	201
202	102	002
021	221	121
110	010	210
122	022	222
211	111	011
220	120	020

(*a*) Assignment of the treatment combinations to blocks



(*b*) Geometric view

Figure 9-7 The 3^3 design in three blocks with AB^2C^2 confounded.

Table 9-5 Analysis of Variance for a 3^3 Design with AB^2C^2 Confounded

Source of Variation	Degrees of Freedom
Blocks (AB^2C^2)	2
A	2
B	2
C	2
AB	4
AC	4
BC	4
Error ($ABC + AB^2C + ABC^2$)	6
Total	26

The analysis of variance for this design is shown in Table 9-5. Using this confounding scheme, information on all the main effects and two-factor interactions is available. The remaining components of the three-factor interaction (ABC, AB^2C, and ABC^2) are combined as an estimate of error. The sum of squares for those three components could be obtained by subtraction. In general, for the 3^k design in three blocks, we would always select a component of the highest-order interaction to confound with blocks. The remaining unconfounded components of this interaction could be obtained by computing the k-factor interaction in the usual way and subtracting from this quantity the sum of squares for blocks.

9-2.2 The 3^k Factorial Design in Nine Blocks

In some experimental situations it may be necessary to confound the 3^k design in nine blocks. Thus, eight degrees of freedom will be confounded with blocks. To construct these designs, we choose *two* components of interaction and, as a result, two more will be confounded automatically, yielding the required eight degrees of freedom. These two are the generalized interactions of the two effects originally chosen. In the 3^k system, the **generalized interactions** of two effects (e.g., P and Q) are defined as PQ and PQ^2 (or P^2Q).

The two components of interaction initially chosen yield *two* defining contrasts

$$\begin{aligned} L_1 &= \alpha_1 x_1 + \alpha_2 x_2 + \cdots + \alpha_k x_k = u \pmod 3 \qquad u = 0, 1, 2 \\ L_2 &= \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k = h \pmod 3 \qquad h = 0, 1, 2 \end{aligned} \tag{9-3}$$

where $\{\alpha_i\}$ and $\{\beta_j\}$ are the exponents in the first and second generalized interactions, respectively, with the convention that the first nonzero α_i and β_j are unity. The defining contrasts in Equation 9-3 imply nine simultaneous equations specified by the pair of values for L_1 and L_2. Treatment combinations having the same pair of values for (L_1, L_2) are assigned to the same block.

The principal block consists of treatment combinations satisfying $L_1 = L_2 = 0 \pmod 3$. The elements of this block form a group with respect to addition modulus 3; thus, the scheme given in Section 9-2.1 can be used to generate the blocks.

As an example, consider the 3^4 factorial design confounded in nine blocks of nine runs each. Suppose we choose to confound ABC and AB^2D^2. Their generalized interactions

$$(ABC)(AB^2D^2) = A^2B^3CD^2 = (A^2B^3CD^2)^2 = AC^2D$$
$$(ABC)(AB^2D^2)^2 = A^3B^5CD^4 = B^2CD = (B^2CD)^2 = BC^2D^2$$

are also confounded with blocks. The defining contrasts for ABC and AB^2D^2 are

$$L_1 = x_1 + x_2 + x_3$$
$$L_2 = x_1 + 2x_2 + 2x_4 \tag{9-4}$$

The nine blocks may be constructed by using the defining contrasts (Equation 9-4) and the group-theoretic property of the principal block. The design is shown in Figure 9-8.

For the 3^k design in nine blocks, there will be four components of interaction confounded. The remaining unconfounded components of these interactions can be determined by subtracting the sum of squares for the confounded component from the sum of squares for the entire interaction. The method described in Section 9-1.3 may be useful in computing the components of interaction.

9-2.3 The 3^k Factorial Design in 3^p Blocks

The 3^k factorial design may be confounded in 3^p blocks of 3^{k-p} observations each, where $p < k$. The procedure is to select p independent effects to be confounded with blocks. As a result, exactly $(3^p - 2p - 1)/2$ other effects are automatically confounded. These effects are the generalized interactions of those effects originally chosen.

As an illustration, consider a 3^7 design to be confounded in 27 blocks. Because $p = 3$, we would select three independent components of interaction and automatically confound $[3^3 - 2(3) - 1]/2 = 10$ others. Suppose we choose ABC^2DG, BCE^2F^2G, and $BDEFG$. Three defining contrasts can be constructed from these effects, and the 27 blocks

Block 1	Block 2	Block 3	Block 4	Block 5	Block 6	Block 7	Block 8	Block 9
0000	0001	2000	0200	0020	0010	1000	0100	0002
0122	0120	2122	0022	0112	0102	1122	0222	0121
0211	0212	2211	0111	0201	0221	1211	0011	0210
1021	1022	0021	0221	1011	1001	2021	1121	1020
1110	1111	0110	1010	1100	1120	2110	1210	1112
1202	1200	0202	1102	1222	1212	2202	1002	1201
2012	2010	1012	2212	2002	2022	0012	2112	2011
2101	2012	1101	2001	2121	2111	0101	2201	2100
2220	2221	1220	2120	2210	2200	0220	2020	2222
$(L_1, L_2) = (0,0)$	(0,1)	(2,2)	(2,0)	(2,1)	(1,2)	(1,1)	(1,0)	(0,2)

Figure 9-8 The 3^4 design in nine blocks with ABC, AB^2D^2, AC^2D, and BC^2D^2 confounded.

can be generated by the methods previously described. The other 10 effects confounded with blocks are

$$(ABC^2DG)(BCE^2F^2G) = AB^2DE^2F^2G^2$$
$$(ABC^2DG)(BCE^2F^2G)^2 = AB^3C^4DE^4F^4G^3 = ACDEF$$
$$(ABC^2DG)(BDEFG) = AB^2C^2D^2EFG^2$$
$$(ABC^2DG)(BDEFG)^2 = AB^3C^2D^3E^2F^2G^3 = AC^2E^2F^2$$
$$(BCE^2F^2G)(BDEFG) = B^2CDE^3F^3G^2 = BC^2D^2G$$
$$(BCE^2F^2G)(BDEFG)^2 = B^3CD^2E^4F^4G^3 = CD^2EF$$
$$(ABC^2DG)(BCE^2F^2G)(BDEFG) = AB^3C^3D^2E^3F^3G^3 = AD^2$$
$$(ABC^2DG)^2(BCE^2F^2G)(BDEFG) = A^2B^4C^5D^3G^4 = AB^2CG^2$$
$$(ABC^2DG)(BCE^2F^2G)^2(BDEFG) = ABCD^2E^2F^2G$$
$$(ABC^2DG)(BCE^2F^2G)(BDEFG)^2 = ABC^3D^3E^4F^4G^4 = ABEFG$$

This is a huge design requiring $3^7 = 2187$ observations arranged in 27 blocks of 81 observations each.

9-3 FRACTIONAL REPLICATION OF THE 3^k FACTORIAL DESIGN

The concept of fractional replication can be extended to the 3^k factorial designs. Because a complete replicate of the 3^k design can require a rather large number of runs even for moderate values of k, fractional replication of these designs is of interest. As we shall see, however, some of these designs have unattractive alias structures.

9-3.1 The One-Third Fraction of the 3^k Factorial Design

The largest fraction of the 3^k design is a one-third fraction containing 3^{k-1} runs. Consequently, we refer to this as a 3^{k-1} fractional factorial design. To construct a 3^{k-1} fractional factorial design select a two-degrees-of-freedom component of interaction (generally, the highest-order interaction) and partition the *full* 3^k design into three blocks. Each of the three resulting blocks is a 3^{k-1} fractional design, and any one of the blocks may be selected for use. If $AB^{\alpha_2}C^{\alpha_3}\cdots K^{\alpha_k}$ is the component of interaction used to define the blocks, then $I = AB^{\alpha_2}C^{\alpha_3}\cdots K^{\alpha_k}$ is called the **defining relation** of the fractional factorial design. Each main effect or component of interaction estimated from the 3^{k-1} design has two aliases, which may be found by multiplying the effect by *both* I and I^2 modulus 3.

As an example, consider a one-third fraction of the 3^3 design. We may select any component of the ABC interaction to construct the design, that is, ABC, AB^2C, ABC^2, or AB^2C^2. Thus, there are actually 12 *different* one-third fractions of the 3^3 design defined by

$$x_1 + \alpha_2 x_2 + \alpha_3 x_3 = u \pmod 3$$

where $\alpha = 1$ or 2 and $u = 0$, 1, or 2. Suppose we select the component of AB^2C^2. Each fraction of the resulting 3^{3-1} design will contain exactly $3^2 = 9$ treatment combinations that must satisfy

$$x_1 + 2x_2 + 2x_3 = u \pmod 3$$

where $u = 0$, 1, or 2. It is easy to verify that the three one-third fractions are as shown in Figure 9-9.

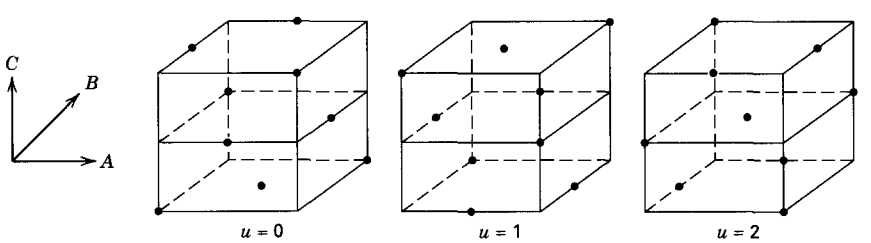
If any one of the 3^{3-1} designs in Figure 9-9 is run, the resulting alias structure is

$$
\begin{aligned}
A &= A(AB^2C^2) = A^2B^2C^2 = ABC \\
A &= A(AB^2C^2)^2 = A^3B^4C^4 = BC \\
B &= B(AB^2C^2) = AB^3C^2 = AC^2 \\
B &= B(AB^2C^2)^2 = A^2B^5C^4 = ABC^2 \\
C &= C(AB^2C^2) = AB^2C^3 = AB^2 \\
C &= C(AB^2C^2)^2 = A^2B^4C^5 = AB^2C \\
AB &= AB(AB^2C^2) = A^2B^3C^2 = AC \\
AB &= AB(AB^2C^2)^2 = A^3B^5C^4 = BC^2
\end{aligned}
$$

Consequently, the four effects that are actually estimated from the eight degrees of freedom in the design are $A + BC + ABC$, $B + AC^2 + ABC^2$, $C + AB^2 + AB^2C$, and $AB + AC + BC^2$. This design would be of practical value only if all the interactions were small relative to the main effects. Because the main effects are aliased with two-factor interactions, this is a resolution III design. Notice how complex the alias relationships are in this design. Each main effect is aliased with a *component* of interaction. If, for example, the two-factor interaction BC is large, this will potentially distort the estimate of the main effect of A and make the $AB + AC + BC^2$ effect very difficult to interpret. It is very difficult to see how this design could be useful unless we assume that all interactions are negligible.

Design 1 $u = 0$	Design 1 $u = 1$	Design 1 $u = 2$
000	100	200
012	112	212
101	201	001
202	002	102
021	121	221
110	210	010
122	222	022
211	011	111
220	020	120

(*a*) Treatment combinations



(*b*) Geometric view

Figure 9-9 The three one-third fractions of the 3^3 design with defining relation $I = AB^2C^2$.

Before leaving the 3_{III}^{3-1} design, note that for the design with $u = 0$ (see Figure 9-9) if we let A denote the row and B denote the column, then the design can be written as

000	012	021
101	110	122
202	211	220

which is a 3×3 Latin square. The assumption of negligible interactions required for unique interpretations of the 3_{III}^{3-1} design is paralleled in the Latin square design. However, the two designs arise from different motives, one as a consequence of fractional replication and the other from randomization restrictions. From Table 4-13 we observe that there are only twelve 3×3 Latin squares and that each one corresponds to one of the twelve different 3^{3-1} fractional factorial designs.

The treatment combinations in a 3^{k-1} design with the defining relation $I = AB^{\alpha_2}C^{\alpha_3} \cdots K^{\alpha_k}$ can be constructed using a method similar to that employed in the 2^{k-p} series. First, write down the 3^{k-1} runs for a **full** three-level factorial design in $k - 1$ factors, with the usual 0, 1, 2 notation. This is the **basic design** in the terminology of Chapter 8. Then introduce the kth factor by equating its levels x_k to the appropriate component of the highest-order interaction, say $AB^{\alpha_2}C^{\alpha_3} \cdots (K-1)^{\alpha_{k-1}}$, through the relationship

$$x_k = \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_{k-1} x_{k-1} \tag{9-5}$$

where $\beta_i = (3 - \alpha_k)\alpha_i \pmod 3$ for $1 \leq i \leq k - 1$. This yields a design of the highest possible resolution.

As an illustration, we use this method to generate the 3_{IV}^{4-1} design with the defining relation $I = AB^2CD$ shown in Table 9-6. It is easy to verify that the first three digits of each treatment combination in this table are the 27 runs of a full 3^3 design. This is the basic design. For AB^2CD, we have $\alpha_1 = \alpha_3 = \alpha_4 = 1$ and $\alpha_2 = 2$. This implies that $\beta_1 = (3 - 1)\alpha_1 \pmod 3 = (3 - 1)(1) = 2$, $\beta_2 = (3 - 1)\alpha_2 \pmod 3 = (3 - 1)(2) = 4 = 1 \pmod 3$, and $\beta_3 = (3 - 1)\alpha_3 \pmod 3 = (3 - 1)(1) = 2$. Thus, Equation 9-5 becomes

$$x_4 = 2x_1 + x_2 + 2x_3 \tag{9-6}$$

The levels of the fourth factor satisfy Equation 9-6. For example, we have $2(0) + 1(0) + 2(0) = 0$, $2(0) + 1(1) + 2(0) = 1$, $2(1) + 1(1) + 2(0) = 3 = 0$, and so on.

The resulting 3_{IV}^{4-1} design has 26 degrees of freedom that may be used to compute

Table 9-6 A 3_{IV}^{4-1} Design with $I = AB^2CD$

0000	0012	2221
0101	0110	0021
1100	0211	0122
1002	1011	0220
0202	1112	1020
1201	1210	1121
2001	2010	1222
2102	2111	2022
2200	2212	2120

the sums of squares for the 13 main effects and components of interactions (and their aliases). The aliases of any effect are found in the usual manner; for example, the aliases of A are $A(AB^2CD) = ABC^2D^2$ and $A(AB^2CD)^2 = BC^2D^2$. One may verify that the four main effects are clear of any two-factor interaction components, but that some two-factor interaction components are aliased with each other. Once again, we notice the complexity of the alias structure. If any two-factor interactions are large, it will likely be very difficult to isolate them with this design.

The statistical analysis of a 3^{k-1} design is accomplished by the usual analysis of variance procedures for factorial experiments. The sums of squares for the components of interaction may be computed as in Section 9-1. Remember when interpreting results that the components of interactions have no practical interpretation.

9-3.2 Other 3^{k-p} Fractional Factorial Designs

For moderate to large values of k, even further fractionation of the 3^k design is potentially desirable. In general, we may construct a $(\frac{1}{3})^p$ fraction of the 3^k design for $p < k$, where the fraction contains 3^{k-p} runs. Such a design is called a 3^{k-p} fractional factorial design. Thus, a 3^{k-2} design is a one-ninth fraction, a 3^{k-3} design is a one–twenty-seventh fraction, and so on.

The procedure for constructing a 3^{k-p} fractional factorial design is to select p components of interaction and use these effects to partition the 3^k treatment combinations into 3^p blocks. Each block is then a 3^{k-p} fractional factorial design. The defining relation I of any fraction consists of the p effects initially chosen and their $(3^p - 2p - 1)/2$ generalized interactions. The alias of any main effect or component of interaction is produced by multiplication modulus 3 of the effect by I and I^2.

We may also generate the runs defining a 3^{k-p} fractional factorial design by first writing down the treatment combinations of a full 3^{k-p} factorial design and then introducing the additional p factors by equating them to components of interaction, as we did in Section 9-3.1.

We illustrate the procedure by constructing a 3^{4-2} design, that is, a one-ninth fraction of the 3^4 design. Let AB^2C and BCD be the two components of interaction chosen to construct the design. Their generalized interactions are $(AB^2C)(BCD) = AC^2D$ and $(AB^2C)(BCD)^2 = ABD^2$. Thus, the defining relation for this design is $I = AB^2C = BCD = AC^2D = ABD^2$, and the design is of resolution III. The nine treatment combinations in the design are found by writing down a 3^2 design in the factors A and B, and then adding two new factors by setting

$$x_3 = 2x_1 + x_2$$
$$x_4 = 2x_2 + 2x_3$$

Table 9-7 A 3^{4-2}_{III} Design with $I = AB^2C$ and $I = BCD$

0000	0111	0222
1021	1102	1210
2012	2120	2201

Table 9-8 Alias Structure for the 3^{4-2}_{III} Design in Table 9-7

Effect	Aliases							
	I				I^2			
A	ABC^2	$ABCD$	ACD^2	AB^2D	BC^2	$AB^2C^2D^2$	CD^2	BD^2
B	AC	BC^2D^2	ABC^2D	AB^2D^2	ABC	CD	AB^2C^2D	AD^2
C	AB^2C^2	BC^2D	AD	$ABCD^2$	AB^2	BD	ACD	ABC^2D^2
D	AB^2CD	BCD^2	AC^2D^2	AB	AB^2CD^2	BC	AC^2	ABD

This is equivalent to using AB^2C and BCD to partition the full 3^4 design into nine blocks and then selecting one of these blocks as the desired fraction. The complete design is shown in Table 9-7 on the facing page.

This design has eight degrees of freedom that may be used to estimate four main effects and their aliases. The aliases of any effect may be found by multiplying the effect modulus 3 by AB^2C, BCD, AC^2D, ABD^2, and their squares. The complete alias structure for the design is given in Table 9-8.

From the alias structure, we see that this design is useful only in the absence of interaction. Furthermore, if A denotes the rows and B denotes the columns, then from examining Table 9-7 we see that the 3^{4-2}_{III} design is also a Graeco–Latin square.

The publication by Connor and Zelen (1959) contains an extensive selection of designs for $4 \leq k \leq 10$. This pamphlet was prepared for the National Bureau of Standards and is the most complete table of fractional 3^{k-p} plans available.

In this section, we have noted several times the complexity of the alias relationships in 3^{k-p} fractional factorial designs. In general, if k is moderately large, say $k \geq 4$ or 5, the size of the 3^k design will drive most experimenters to consider fairly small fractions. Unfortunately, these designs have alias relationships that involve the **partial aliasing** of two-degrees-of-freedom components of interaction. This, in turn, results in a design that will be difficult if not impossible to interpret if interactions are not negligible. Furthermore, there are no simple augmentation schemes (such as fold over) that can be used to combine two or more fractions to isolate significant interactions. The 3^k design is often suggested as appropriate when curvature is present. However, there are more efficient alternatives (see Chapter 11). For these reasons, I feel that the 3^{k-p} fractional factorial designs are solutions looking for a problem—they are not generally good designs.

9-4 FACTORIALS WITH MIXED LEVELS

We have emphasized factorial and fractional factorial designs in which all the factors have the same number of levels. The two-level system discussed in Chapters 6, 7, and 8 is particularly useful. The three-level system presented earlier in this chapter is much less useful because the designs are relatively large even for a modest number of factors, and most of the small fractions have complex alias relationships that would require very restrictive assumptions regarding interactions to be useful.

It is our belief that the two-level factorial and fractional factorial designs should be the cornerstone of industrial experimentation for product and process development, troubleshooting, and improvement. There are, however, some situations in which it is necessary to include a factor (or a few factors) that has more than two levels. This usually occurs when there are both quantitative and qualitative factors in the experiment, and

Table 9-9 Use of Two-Level Factors to Form a Three-Level Factor

Two-Level Factors		Three-Level Factor
B	C	X
−	−	x_1
+	−	x_2
−	+	x_2
+	+	x_3

the qualitative factor has (say) three levels. If all factors are quantitative, then two-level designs with center points should be employed. In this section we show how some three- and four-level factors can be accommodated in a 2^k design.

9-4.1 Factors at Two and Three Levels

Designs in which some factors have two levels and other factors have three levels can be derived from the table of plus and minus signs for the usual 2^k design. The general procedure is best illustrated with an example. Suppose we have two variables, with A at two levels and X at three levels. Consider a table of plus and minus signs for the usual eight-run 2^3 design. The signs in columns B and C have the pattern shown on the left side of Table 9-9. Let the levels of X be represented by x_1, x_2, and x_3. The right side of Table 9-9 shows how the sign patterns for B and C are combined to form the levels of the three-level factor.

Now factor X has two degrees of freedom and if the factor is quantitative it can be partitioned into a linear and a quadratic component, each component having one degree of freedom. Table 9-10 shows a 2^3 design with the columns labeled to show the actual effects that they estimate, with X_L and X_Q denoting the linear and quadratic effects of X, respectively. Note that the linear effect of X is the sum of the two effect estimates computed from the columns usually associated with B and C and that the effect of A can only be computed from the runs where X is at either the low or high levels, namely runs 1, 2, 7, and 8. Similarly, the $A \times X_L$ effect is the sum of the two effects that would be computed from the columns usually labeled AB and AC. Furthermore, note that runs 3

Table 9-10 One 2-Level and One 3-Level Factor in a 2^3 Design

	A	X_L	X_L	$A \times X_L$	$A \times X_L$	X_Q	$A \times X_Q$	Actual Treatment Combinations	
Run	A	B	C	AB	AC	BC	ABC	A	X
1	−	−	−	+	+	+	−	Low	Low
2	+	−	−	−	−	+	+	High	Low
3	−	+	−	−	+	−	+	Low	Med
4	+	+	−	+	−	−	−	High	Med
5	−	−	+	+	−	−	+	Low	Med
6	+	−	+	−	+	−	−	High	Med
7	−	+	+	−	−	+	−	Low	High
8	+	+	+	+	+	+	+	High	High

Table 9-11 Analysis of Variance for the Design in Table 9-10

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square
A	SS_A	1	MS_A
X ($X_L + X_Q$)	SS_X	2	MS_B
AX ($A \times X_L + A \times X_Q$)	SS_{AX}	2	MS_{AX}
Error (from runs 3 and 5 and runs 4 and 6)	SS_E	2	MS_E
Total	SS_T	7	

and 5 are replicates. Therefore, a one-degree-of-freedom estimate of error can be made using these two runs. Similarly, runs 4 and 6 are replicates, and this would lead to a second one-degree-of-freedom estimate of error. The average variance at these two pairs of runs could be used as a mean square for error with two degrees of freedom. The complete analysis of variance is summarized in Table 9-11.

If we are willing to assume that the two-factor and higher interactions are negligible, we can convert the design in Table 9-10 into a resolution III fraction with up to four two-level factors and a single three-level factor. This would be accomplished by associating the two-level factors with columns A, AB, AC, and ABC. Column BC cannot be used for a two-level factor because it contains the quadratic effect of the three-level factor X.

This same procedure can be applied to the 16-, 32-, and 64-run 2^k designs. For 16 runs, it is possible to construct resolution V fractional factorials with two two-level factors and either two or three factors at three levels. A 16-run resolution V fraction can also be obtained with 3 two-level factors and one three-level factor. If we include four two-level factors and a single three-level factor in 16 runs, the design will be of resolution III. The 32- and 64-run designs allow similar arrangements. For additional discussion of some of these designs, see Addleman (1962).

9-4.2 Factors at Two and Four Levels

It is very easy to accommodate a four-level factor in a 2^k design. The procedure for doing this involves using two two-level factors to represent the four-level factor. For example, suppose that A is a four-level factor with levels a_1, a_2, a_3, and a_4. Consider two columns of the usual table of plus and minus signs, say columns P and Q. The pattern of signs in these two columns is as shown on the left side of Table 9-12. The right side of this table shows how these four sign patterns would correspond to the four levels of factor A. The

Table 9-12 Four-Level Factor A Expressed as 2 Two-Level Factors

	Two-Level Factors		Four-Level Factor
Run	P	Q	A
1	−	−	a_1
2	+	−	a_2
3	−	+	a_3
4	+	+	a_4

Table 9-13 A Single Four-Level Factor and 2 Two-Level Factors in 16 Runs

Run	(*A*	*B*)	= *X*	*C*	*D*	*AB*	*AC*	*BC*	*ABC*	*AD*	*BD*	*ABD*	*CD*	*ACD*	*BCD*	*ABCD*
1	−	−	x_1	−	−	+	+	+	−	+	+	−	+	−	−	+
2	+	−	x_2	−	−	−	−	+	+	−	+	+	+	+	−	−
3	−	+	x_3	−	−	−	+	−	+	+	−	+	+	−	+	−
4	+	+	x_4	−	−	+	−	−	−	−	−	−	+	+	+	+
5	−	−	x_1	+	−	+	−	−	+	+	+	−	−	+	+	−
6	+	−	x_2	+	−	−	+	−	−	−	+	+	−	−	+	+
7	−	+	x_3	+	−	−	−	+	−	+	−	+	−	+	−	+
8	+	+	x_4	+	−	+	+	+	+	−	−	−	−	−	−	−
9	−	−	x_1	−	+	+	+	+	−	−	−	+	−	+	+	−
10	+	−	x_2	−	+	−	−	+	+	+	−	−	−	−	+	+
11	−	+	x_3	−	+	−	+	−	+	−	+	−	−	+	−	+
12	+	+	x_4	−	+	+	−	−	−	+	+	+	−	−	−	−
13	−	−	x_1	+	+	+	−	−	+	−	−	+	+	−	−	+
14	+	−	x_2	+	+	−	+	−	−	+	−	−	+	+	−	−
15	−	+	x_3	+	+	−	−	+	−	−	+	−	+	−	+	−
16	+	+	x_4	+	+	+	+	+	+	+	+	+	+	+	+	+

effects represented by columns P and Q and the PQ interaction are mutually orthogonal and correspond to the three-degrees-of-freedom A effect.

To illustrate this idea more completely, suppose that we have one four-level factor and two two-level factors and that we need to estimate all the main effects and interactions involving these factors. This can be done with a 16-run design. Table 9-13 (on the facing page) shows the usual table of plus and minus signs for the 16-run 2^4 design, with columns A and B used to form the four-level factor, say X, with levels x_1, x_2, x_3, and x_4. Sums of squares would be calculated for each column $A, B, \ldots, ABCD$ just as in the usual 2^k system. Then the sums of squares for all factors X, C, D, and their interactions are formed as follows:

$$
\begin{aligned}
SS_X &= SS_A + SS_B + SS_{AB} && \text{(3 degrees of freedom)} \\
SS_C &= SS_C && \text{(1 degree of freedom)} \\
SS_D &= SS_D && \text{(1 degree of freedom)} \\
SS_{CD} &= SS_{CD} && \text{(1 degree of freedom)} \\
SS_{XC} &= SS_{AC} + SS_{BC} + SS_{ABC} && \text{(3 degrees of freedom)} \\
SS_{XD} &= SS_{AD} + SS_{BD} + SS_{ABD} && \text{(3 degrees of freedom)} \\
SS_{XCD} &= SS_{ACD} + SS_{BCD} + SS_{ABCD} && \text{(3 degrees of freedom)}
\end{aligned}
$$

This could be called a 4×2^2 design. If we are willing to ignore two-factor interactions, up to nine additional two-level factors can be associated with the two-factor interaction (except AB), three-factor interaction, and four-factor interaction columns.

9-5 PROBLEMS

9-1. The effects of developer strength (A) and development time (B) on the density of photographic plate film are being studied. Three strengths and three times are used, and four replicates of a 3^2 factorial experiment are run. The data from this experiment follow. Analyze the data using the standard methods for factorial experiments.

	Development Time (minutes)					
Developer Strength	10		14		18	
1	0	2	1	3	2	5
	5	4	4	2	4	6
2	4	6	6	8	9	10
	7	5	7	7	8	5
3	7	10	10	10	12	10
	8	7	8	7	9	8

9-2. Compute the I and J components of the two-factor interaction in Problem 9-1.

9-3. An experiment was performed to study the effect of three different types of 32-ounce bottles (A) and three different shelf types (B)—smooth permanent shelves, end-aisle displays with grilled shelves, and beverage coolers—on the time it takes to stock ten 12-bottle cases on the shelves. Three workers (factor C) were employed in the experiment, and two replicates of a 3^3 factorial design were run. The observed time data are shown in the following table. Analyze the data and draw conclusions.

		Replicate I			Replicate II		
Worker	Bottle Type	Permanent	End Aisle	Cooler	Permanent	End Aisle	Cooler
	Plastic	3.45	4.14	5.80	3.36	4.19	5.23
1	28-mm glass	4.07	4.38	5.48	3.52	4.26	4.85
	38-mm glass	4.20	4.26	5.67	3.68	4.37	5.58
	Plastic	4.80	5.22	6.21	4.40	4.70	5.88
2	28-mm glass	4.52	5.15	6.25	4.44	4.65	6.20
	38-mm glass	4.96	5.17	6.03	4.39	4.75	6.38
	Plastic	4.08	3.94	5.14	3.65	4.08	4.49
3	28-mm glass	4.30	4.53	4.99	4.04	4.08	4.59
	38-mm glass	4.17	4.86	4.85	3.88	4.48	4.90

9-4. A medical researcher is studying the effect of lidocaine on the enzyme level in the heart muscle of beagle dogs. Three different commercial brands of lidocaine (A), three dosage levels (B), and three dogs (C) are used in the experiment, and two replicates of a 3^3 factorial design are run. The observed enzyme levels follow. Analyze the data from this experiment.

		Replicate I			Replicate II		
		Dog			Dog		
Lidocaine Brand	Dosage Strength	1	2	3	1	2	3
	1	96	84	85	84	85	86
1	2	94	99	98	95	97	90
	3	101	106	98	105	104	103
	1	85	84	86	80	82	84
2	2	95	98	97	93	99	95
	3	108	114	109	110	102	100
	1	84	83	81	83	80	79
3	2	95	97	93	92	96	93
	3	105	100	106	102	111	108

9-5. Compute the I and J components of the two-factor interactions for Example 10-1.

9-6. An experiment is run in a chemical process using a 3^2 factorial design. The design factors are temperature and pressure, and the response variable is yield. The data that result from this experiment are shown below:

	Pressure, psig		
Temperature, °C	100	120	140
80	47.58, 48.77	64.97, 69.22	80.92, 72.60
90	51.86, 82.43	88.47, 84.23	93.95, 88.54
100	71.18, 92.77	96.57, 88.72	76.58, 83.04

(a) Analyze the data from this experiment by conducting an analysis of variance. What conclusions can you draw?

(b) Graphically analyze the residuals. Are there any concerns about underlying assumptions or model adequacy?

(c) Verify that if we let the low, medium, and high levels of both factors in this design take on the levels -1, 0, and $+1$, then a least squares fit to a second-order model for yield is

$$\hat{y} = 86.81 + 10.4x_1 + 8.42x_2 - 7.17x_1^2 - 7.86x_2^2 - 7.69x_1x_2$$

(d) Confirm that the model in part (c) can be written in terms of the natural variables temperature (T) and pressure (P) as

$$\hat{y} = -1335.63 + 18.56T + 8.59P - 0.072T^2 - 0.0196P^2 - 0.0384TP$$

(e) Construct a contour plot for yield as a function of pressure and temperature. Based on examination of this plot, where would you recommend running this process?

9-7. (a) Confound a 3^3 design in three blocks using the ABC^2 component of the three-factor interaction. Compare your results with the design in Figure 9-7.

(b) Confound a 3^3 design in three blocks using the AB^2C component of the three-factor interaction. Compare your results with the design in Figure 9-7.

(c) Confound a 3^3 design in three blocks using the ABC component of the three-factor interaction. Compare your results with the design in Figure 9-7.

(d) After looking at the designs in parts (a), (b), and (c) and Figure 9-7, what conclusions can you draw?

9-8. Confound a 3^4 design in three blocks using the AB^2CD component of the four-factor interaction.

9-9. Consider the data from the first replicate of Problem 9-3. Assuming that all 27 observations could not be run on the same day, set up a design for conducting the experiment over three days with AB^2C confounded with blocks. Analyze the data.

9-10. Outline the analysis of variance table for the 3^4 design in nine blocks. Is this a practical design?

9-11. Consider the data in Problem 9-3. If ABC is confounded in replicate I and ABC^2 is confounded in replicate II, perform the analysis of variance.

9-12. Consider the data from replicate I of Problem 9-3. Suppose that only a one-third fraction of this design with $I = ABC$ is run. Construct the design, determine the alias structure, and analyze the data.

9-13. From examining Figure 9-9, what type of design would remain if after completing the first nine runs, one of the three factors could be dropped?

9-14. Construct a 3^{4-1}_{IV} design with $I = ABCD$. Write out the alias structure for this design.

9-15. Verify that the design in Problem 9-14 is a resolution IV design.

9-16. Construct a 3^{5-2} design with $I = ABC$ and $I = CDE$. Write out the alias structure for this design. What is the resolution of this design?

9-17. Construct a 3^{9-6} design, and verify that it is a resolution III design.

9-18. Construct a 4×2^3 design confounded in two blocks of 16 observations each. Outline the analysis of variance for this design.

9-19. Outline the analysis of variance table for a $2^2 3^2$ factorial design. Discuss how this design may be confounded in blocks.

9-20. Starting with a 16-run 2^4 design, show how two three-level factors can be incorporated in this experiment. How many two-level factors can be included if we want some information on two-factor interactions?

9-21. Starting with a 16-run 2^4 design, show how one three-level factor and three two-level factors can be accommodated and still allow the estimation of two-factor interactions.

9-22. In Problem 8-26, you met Harry and Judy Peterson-Nedry, two friends of the author who have a winery and vineyard in Newberg, Oregon. That problem described the application of two-level fractional factorial designs to their 1985 Pinot Noir product. In 1987, they wanted to conduct another Pinot Noir experiment. The variables for this experiment were

Variable	Levels
Clone of Pinot Noir	Wadenswil, Pommard
Berry size	Small, large
Fermentation temperature	80°F, 85°F, 90/80°F, 90°F
Whole berry	None, 10%
Maceration time	10 days, 21 days
Yeast type	Assmanhau, Champagne
Oak type	Tronçais, Allier

Harry and Judy decided to use a 16-run two-level fractional factorial design, treating the four levels of fermentation temperature as two two-level variables. As in Problem 8-26, they used the rankings from a taste-test panel as the response variable. The design and the resulting average ranks are shown below:

Run	Clone	Berry Size	Ferm. Temp.		Whole Berry	Macer. Time	Yeast Type	Oak Type	Average Rank
1	−	−	−	−	−	−	−	−	4
2	+	−	−	−	−	+	+	+	10
3	−	+	−	−	+	−	+	+	6
4	+	+	−	−	+	+	−	−	9
5	−	−	+	−	+	+	+	−	11
6	+	−	+	−	+	−	−	+	1
7	−	+	+	−	−	+	−	+	15
8	+	+	+	−	−	−	+	−	5
9	−	−	−	+	+	+	−	+	12
10	+	−	−	+	+	−	+	−	2
11	−	+	−	+	−	+	+	−	16
12	+	+	−	+	−	−	−	+	3
13	−	−	+	+	−	−	+	+	8
14	+	−	+	+	−	+	−	−	14
15	−	+	+	+	+	−	−	−	7
16	+	+	+	+	+	+	+	+	13

(a) Describe the aliasing in this design.
(b) Analyze the data and draw conclusions.
(c) What comparisons can you make between this experiment and the 1985 Pinot Noir experiment from Problem 8-26?

9-23. An article by W. D. Baten in the 1956 volume of *Industrial Quality Control* described an experiment to study the effect of three factors on the lengths of steel bars. Each bar was subjected to one of two heat treatment processes and was cut on one of four machines at one of three times during the day (8 a.m., 11 a.m., or 3 p.m.). The coded length data are shown below:

Time of Day	Heat Treatment Process	Machine 1		Machine 2		Machine 3		Machine 4	
8 a.m.	1	6	9	7	9	1	2	6	6
		1	3	5	5	0	4	7	3
	2	4	6	6	5	−1	0	4	5
		0	1	3	4	0	1	5	4

Time of Day	Heat Treatment Process	Machine							
		1		2		3		4	
11 a.m.	1	6	3	8	7	3	2	7	9
		1	−1	4	8	1	0	11	6
	2	3	1	6	4	2	0	9	4
		1	−2	1	3	−1	1	6	3
3 p.m.	1	5	4	10	11	−1	2	10	5
		9	6	6	4	6	1	4	8
	2	6	0	8	7	0	−2	4	3
		3	7	10	0	4	−4	7	0

(a) Analyze the data from this experiment, assuming that the four observations in each cell are replicates.

(b) Analyze the residuals from this experiment. Is there any indication that there is an outlier in one cell? If you find an outlier, remove it and repeat the analysis from part (a). What are your conclusions?

(c) Suppose that the observations in the cells are the lengths (coded) of bars processed together in heat treating and then cut sequentially (that is, in order) on the four machines. Analyze the data to determine the effects of the three factors on mean length.

(d) Calculate the log variance of the observations in each cell. Analyze this response. What conclusions can you draw?

(e) Suppose the time at which a bar is cut really cannot be controlled during routine production. Analyze the average length and the log variance of the length for each of the 12 bars cut at each machine/heat treatment process combination. What conclusions can you draw?

10 Fitting Regression Models

10-1 INTRODUCTION

In many problems there are two or more variables that are related, and it is of interest to model and explore this relationship. For example, in a chemical process the yield of product is related to the operating temperature. The chemical engineer may want to build a model relating yield to temperature and then use the model for prediction, process optimization, or process control.

In general, suppose that there is a single **dependent variable** or **response** y that depends on k **independent** or **regressor variables**, for example, $x_1, x_2, \ldots, x_k$. The relationship between these variables is characterized by a mathematical model called a **regression model**. The regression model is fit to a set of sample data. In some instances, the experimenter knows the exact form of the true functional relationship between y and $x_1, x_2, \ldots, x_k$, say $y = \phi(x_1, x_2, \ldots, x_k)$. However, in most cases, the true functional relationship is unknown, and the experimenter chooses an appropriate function to approximate ϕ. Low-order polynomial models are widely used as approximating functions.

There is a strong interplay between design of experiments and regression analysis. Throughout this book we have emphasized the importance of expressing the results of an experiment quantitatively, in terms of an **empirical model**, to facilitate understanding, interpretation, and implementation. Regression models are the basis for this. On numerous occasions we have shown the regression model that represented the results of an experiment. In this chapter, we present some aspects of fitting these models. More complete presentations of regression are available in Montgomery and Peck (1992) and Myers (1990).

Regression methods are frequently used to analyze data from **unplanned experiments**, such as might arise from observation of uncontrolled phenomena or historical records. Regression methods are also very useful in designed experiments where something has "gone wrong." We will illustrate some of these situations in this chapter.

10-2 LINEAR REGRESSION MODELS

We will focus on fitting linear regression models. To illustrate, suppose that we wish to develop an empirical model relating the viscosity of a polymer to the temperature and the catalyst feed rate. A model that might describe this relationship is

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon \tag{10-1}$$

where y represents the viscosity, x_1 represents the temperature, and x_2 represents the catalyst feed rate. This is a **multiple linear regression model** with two independent variables. We often call the independent variables **predictor variables** or **regressors**. The term *linear* is used because Equation 10-1 is a linear function of the unknown parameters β_0, β_1, and β_2. The model describes a plane in the two-dimensional x_1, x_2 space. The parameter β_0 defines the intercept of the plane. We sometimes call β_1 and β_2 *partial regression coefficients*, because β_1 measures the expected change in y per unit change in x_1 when x_2 is held constant, and β_2 measures the expected change in y per unit change in x_2 when x_1 is held constant.

In general, the response variable y may be related to k regressor variables. The model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \epsilon \tag{10-2}$$

is called a *multiple linear regression model* with k regressor variables. The parameters β_j, $j = 0, 1, \ldots, k$, are called the *regression coefficients*. This model describes a hyperplane in the k-dimensional space of the regressor variables $\{x_j\}$. The parameter β_j represents the expected change in response y per unit change in x_j when all the remaining independent variables x_i $(i \neq j)$ are held constant.

Models that are more complex in appearance than Equation 10-2 may often still be analyzed by multiple linear regression techniques. For example, consider adding an interaction term to the first-order model in two variables, say

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \epsilon \tag{10-3}$$

If we let $x_3 = x_1 x_2$ and $\beta_3 = \beta_{12}$, then Equation 10-3 can be written as

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon \tag{10-4}$$

which is a standard multiple linear regression model with three regressors. Recall that we presented empirical models like Equations 10-2 and 10-4 in several examples in Chapters 6, 7, and 8 to quantitatively express the results of a two-level factorial design. As another example, consider the second-order **response surface model** in two variables:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \epsilon \tag{10-5}$$

If we let $x_3 = x_1^2$, $x_4 = x_2^2$, $x_5 = x_1 x_2$, $\beta_3 = \beta_{11}$, $\beta_4 = \beta_{22}$, and $\beta_5 = \beta_{12}$, then this becomes

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \epsilon \tag{10-6}$$

which is a linear regression model. We have also seen this model in examples earlier in the text. In general, any regression model that is linear in the parameters (the β values) is a linear regression model, regardless of the shape of the response surface that it generates.

In this chapter we will summarize methods for estimating the parameters in multiple linear regression models. This is often called **model fitting**. We will also discuss methods

for testing hypotheses and constructing confidence intervals for these models as well as for checking the adequacy of the model fit. Our focus is primarily on those aspects of regression analysis useful in designed experiments. For more complete presentations of regression, refer to Montgomery and Peck (1992) and Myers (1990).

10-3 ESTIMATION OF THE PARAMETERS IN LINEAR REGRESSION MODELS

The method of least squares is typically used to estimate the regression coefficients in a multiple linear regression model. Suppose that $n > k$ observations on the response variable are available, say $y_1, y_2, \ldots, y_n$. Along with each observed response y_i, we will have an observation on each regressor variable and let x_{ij} denote the ith observation or level of variable x_j. The data will appear as in Table 10-1. We assume that the error term ϵ in the model has $E(\epsilon) = 0$ and $V(\epsilon) = \sigma^2$ and that the $\{\epsilon_i\}$ are uncorrelated random variables.

We may write the model equation (Equation 10-2) in terms of the observations in Table 10-1 as

$$\begin{aligned} y_i &= \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik} + \epsilon_i \\ &= \beta_0 + \sum_{j=1}^{k} \beta_j x_{ij} + \epsilon_i \qquad i = 1, 2, \ldots, n \end{aligned} \tag{10-7}$$

The method of least squares chooses the β's in Equation 10-7 so that the sum of the squares of the errors, ϵ_i, is minimized. The least squares function is

$$\begin{aligned} L &= \sum_{i=1}^{n} \epsilon_i^2 \\ &= \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{k} \beta_j x_{ij} \right)^2 \end{aligned} \tag{10-8}$$

The function L is to be minimized with respect to $\beta_0, \beta_1, \ldots, \beta_k$. The least squares estimators, say $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_k$, must satisfy

$$\left. \frac{\partial L}{\partial \beta_0} \right|_{\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_k} = -2 \sum_{i=1}^{n} \left(y_i - \hat{\beta}_0 - \sum_{j=1}^{k} \hat{\beta}_j x_{ij} \right) = 0 \tag{10-9a}$$

and

$$\left. \frac{\partial L}{\partial \beta_j} \right|_{\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_k} = -2 \sum_{i=1}^{n} \left(y_i - \hat{\beta}_0 - \sum_{j=1}^{k} \hat{\beta}_j x_{ij} \right) x_{ij} = 0 \qquad j = 1, 2, \ldots, k \tag{10-9b}$$

Table 10-1 Data for Multiple Linear Regression

y	x_1	x_2	$\cdots$	x_k
y_1	x_{11}	x_{12}	$\cdots$	x_{1k}
y_2	x_{21}	x_{22}	$\cdots$	x_{2k}
$\vdots$	$\vdots$	$\vdots$		$\vdots$
y_n	x_{n1}	x_{n2}	$\cdots$	x_{nk}

Simplifying Equation 10-9, we obtain

$$\begin{aligned}
n\hat{\beta}_0 + \hat{\beta}_1 \sum_{i=1}^{n} x_{i1} + \hat{\beta}_2 \sum_{i=1}^{n} x_{i2} + \cdots + \hat{\beta}_k \sum_{i=1}^{n} x_{ik} &= \sum_{i=1}^{n} y_i \\
\hat{\beta}_0 \sum_{i=1}^{n} x_{i1} + \hat{\beta}_1 \sum_{i=1}^{n} x_{i1}^2 + \hat{\beta}_2 \sum_{i=1}^{n} x_{i1}x_{i2} + \cdots + \hat{\beta}_k \sum_{i=1}^{n} x_{i1}x_{ik} &= \sum_{i=1}^{n} x_{i1}y_i \\
&\vdots \\
\hat{\beta}_0 \sum_{i=1}^{n} x_{ik} + \hat{\beta}_i \sum_{i=1}^{n} x_{ik}x_{i1} + \hat{\beta}_2 \sum_{i=1}^{n} x_{ik}x_{i2} + \cdots + \hat{\beta}_k \sum_{i=1}^{n} x_{ik}^2 &= \sum_{i=1}^{n} x_{ik}y_i
\end{aligned} \tag{10-10}$$

These equations are called the **least squares normal equations**. Note that there are $p = k + 1$ normal equations, one for each of the unknown regression coefficients. The solution to the normal equations will be the least squares estimators of the regression coefficients $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_k$.

It is simpler to solve the normal equations if they are expressed in matrix notation. We now give a matrix development of the normal equations that parallels the development of Equation 10-10. The model in terms of the observations, Equation 10-7, may be written in matrix notation as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \qquad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix},$$

$$\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} \quad \text{and} \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

In general, $\mathbf{y}$ is an $(n \times 1)$ vector of the observations, $\mathbf{X}$ is an $(n \times p)$ matrix of the levels of the independent variables, $\boldsymbol{\beta}$ is a $(p \times 1)$ vector of the regression coefficients, and $\boldsymbol{\epsilon}$ is an $(n \times 1)$ vector of random errors.

We wish to find the vector of least squares estimators, $\hat{\boldsymbol{\beta}}$, that minimizes

$$L = \sum_{i=1}^{n} \epsilon_i^2 = \boldsymbol{\epsilon}'\boldsymbol{\epsilon} = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Note that L may be expressed as

$$\begin{aligned}
L &= \mathbf{y}'\mathbf{y} - \boldsymbol{\beta}'\mathbf{X}'\mathbf{y} - \mathbf{y}'\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta} \\
&= \mathbf{y}'\mathbf{y} - 2\boldsymbol{\beta}'\mathbf{X}'\mathbf{y} + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta}
\end{aligned} \tag{10-11}$$

because $\boldsymbol{\beta}'\mathbf{X}'\mathbf{y}$ is a (1×1) matrix, or a scalar, and its transpose $(\boldsymbol{\beta}'\mathbf{X}'\mathbf{y})' = \mathbf{y}'\mathbf{X}\boldsymbol{\beta}$ is the same scalar. The least squares estimators must satisfy

$$\left.\frac{\partial L}{\partial \boldsymbol{\beta}}\right|_{\hat{\beta}} = -2\mathbf{X}'\mathbf{y} + 2\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{0}$$

which simplifies to

$$\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{y} \tag{10-12}$$

Equation 10-12 is the matrix form of the least squares normal equations. It is identical to Equation 10-10. To solve the normal equations, multiply both sides of Equation 10-12 by the inverse of $\mathbf{X}'\mathbf{X}$. Thus, the least squares estimator of $\boldsymbol{\beta}$ is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \tag{10-13}$$

It is easy to see that the matrix form of the normal equations is identical to the scalar form. Writing out Equation 10-12 in detail, we obtain

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_{i1} & \sum_{i=1}^{n} x_{i2} & \cdots & \sum_{i=1}^{n} x_{ik} \\ \sum_{i=1}^{n} x_{i1} & \sum_{i=1}^{n} x_{i1}^2 & \sum_{i=1}^{n} x_{i1}x_{i2} & \cdots & \sum_{i=1}^{n} x_{i1}x_{ik} \\ \vdots & \vdots & \vdots & & \vdots \\ \sum_{i=1}^{n} x_{ik} & \sum_{i=1}^{n} x_{ik}x_{i1} & \sum_{i=1}^{n} x_{ik}x_{i2} & \cdots & \sum_{i=1}^{n} x_{ik}^2 \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_{i1}y_i \\ \vdots \\ \sum_{i=1}^{n} x_{ik}y_i \end{bmatrix}$$

If the indicated matrix multiplication is performed, the scalar form of the normal equations (i.e., Equation 10-10) will result. In this form it is easy to see that $\mathbf{X}'\mathbf{X}$ is a $(p \times p)$ symmetric matrix and $\mathbf{X}'\mathbf{y}$ is a $(p \times 1)$ column vector. Note the special structure of the $\mathbf{X}'\mathbf{X}$ matrix. The diagonal elements of $\mathbf{X}'\mathbf{X}$ are the sums of squares of the elements in the columns of $\mathbf{X}$, and the off-diagonal elements are the sums of cross-products of the elements in the columns of $\mathbf{X}$. Furthermore, note that the elements of $\mathbf{X}'\mathbf{y}$ are the sums of cross-products of the columns of $\mathbf{X}$ and the observations $\{y_i\}$.

The fitted regression model is

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}} \tag{10-14}$$

In scalar notation, the fitted model is

$$\hat{y}_i = \hat{\beta}_0 + \sum_{j=1}^{k} \hat{\beta}_j x_{ij} \qquad i = 1, 2, \ldots, n$$

The difference between the actual observation y_i and the corresponding fitted value $\hat{y}_i$ is the **residual**, say $e_i = y_i - \hat{y}_i$. The $(n \times 1)$ vector of residuals is denoted by

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} \tag{10-15}$$

Estimating σ^2

It is also usually necessary to estimate σ^2. To develop an estimator of this parameter, consider the sum of squares of the residuals, say

$$\begin{aligned} SS_E &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n} e_i^2 \\ &= \mathbf{e}'\mathbf{e} \end{aligned}$$

Substituting $\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} = \mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}$, we have

$$\begin{aligned} SS_E &= (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})'(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \\ &= \mathbf{y}'\mathbf{y} - \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} - \mathbf{y}'\mathbf{X}\hat{\boldsymbol{\beta}} + \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} \\ &= \mathbf{y}'\mathbf{y} - 2\hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} + \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} \end{aligned}$$

Because $\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{y}$, this last equation becomes

$$SS_E = \mathbf{y}'\mathbf{y} - \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} \tag{10-16}$$

Equation 10-16 is called the **error** or **residual sum of squares**, and it has $n - p$ degrees of freedom associated with it. It can be shown that

$$E(SS_E) = \sigma^2(n - p)$$

so an unbiased estimator of σ^2 is given by

$$\hat{\sigma}^2 = \frac{SS_E}{n - p} \tag{10-17}$$

Properties of the Estimators

The method of least squares produces an unbiased estimator of the parameter $\boldsymbol{\beta}$ in the linear regression model. This may be easily demonstrated by taking the expected value of $\hat{\boldsymbol{\beta}}$ as follows:

$$\begin{aligned} E(\hat{\boldsymbol{\beta}}) &= E[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}] \\ &= E[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'(\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon})] \\ &= E[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\boldsymbol{\beta} + (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\epsilon}] \\ &= \boldsymbol{\beta} \end{aligned}$$

because $E(\boldsymbol{\epsilon}) = \mathbf{0}$ and $(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X} = \mathbf{I}$. Thus, $\hat{\boldsymbol{\beta}}$ is an unbiased estimator of $\boldsymbol{\beta}$.

The variance property of $\hat{\boldsymbol{\beta}}$ is expressed in the **covariance matrix**:

$$\text{Cov}(\hat{\boldsymbol{\beta}}) \equiv E\{[\hat{\boldsymbol{\beta}} - E(\hat{\boldsymbol{\beta}})][\hat{\boldsymbol{\beta}} - E(\hat{\boldsymbol{\beta}})]'\} \tag{10-18}$$

which is just a symmetric matrix whose ith main diagonal element is the variance of the individual regression coefficient $\hat{\beta}_i$ and whose (ij)th element is the covariance between $\hat{\beta}_i$ and $\hat{\beta}_j$. The covariance matrix of $\hat{\boldsymbol{\beta}}$ is

$$\text{Cov}(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1} \tag{10-19}$$

EXAMPLE 10-1

Sixteen observations on the viscosity of a polymer (y) and two process variables—reaction temperature (x_1) and catalyst feed rate (x_2)—are shown in Table 10-2 on the next page. We will fit a multiple linear regression model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

Table 10-2 Viscosity Data for Example 10-1 (viscosity in centistokes @ 100°C)

Observation	Temperature (x_1, °C)	Catalyst Feed Rate (x_2, lb/h)	Viscosity
1	80	8	2256
2	93	9	2340
3	100	10	2426
4	82	12	2293
5	90	11	2330
6	99	8	2368
7	81	8	2250
8	96	10	2409
9	94	12	2364
10	93	11	2379
11	97	13	2440
12	95	11	2364
13	100	8	2404
14	85	12	2317
15	86	9	2309
16	87	12	2328

to these data. The $\mathbf{X}$ matrix and $\mathbf{y}$ vector are

$$\mathbf{X} = \begin{bmatrix} 1 & 80 & 8 \\ 1 & 93 & 9 \\ 1 & 100 & 10 \\ 1 & 82 & 12 \\ 1 & 90 & 11 \\ 1 & 99 & 8 \\ 1 & 81 & 8 \\ 1 & 96 & 10 \\ 1 & 94 & 12 \\ 1 & 93 & 11 \\ 1 & 97 & 13 \\ 1 & 95 & 11 \\ 1 & 100 & 8 \\ 1 & 85 & 12 \\ 1 & 86 & 9 \\ 1 & 87 & 12 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 2256 \\ 2340 \\ 2426 \\ 2293 \\ 2330 \\ 2368 \\ 2250 \\ 2409 \\ 2364 \\ 2379 \\ 2440 \\ 2364 \\ 2404 \\ 2317 \\ 2309 \\ 2328 \end{bmatrix}$$

The $\mathbf{X}'\mathbf{X}$ matrix is

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 80 & 93 & \cdots & 87 \\ 8 & 9 & \cdots & 12 \end{bmatrix} \begin{bmatrix} 1 & 80 & 8 \\ 1 & 93 & 9 \\ \vdots & \vdots & \vdots \\ 1 & 87 & 12 \end{bmatrix}$$

$$= \begin{bmatrix} 16 & 1458 & 164 \\ 1458 & 133{,}560 & 14{,}946 \\ 164 & 14{,}946 & 1{,}726 \end{bmatrix}$$

and the $\mathbf{X}'\mathbf{y}$ vector is

$$\mathbf{X}'\mathbf{y} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 80 & 93 & \cdots & 87 \\ 8 & 9 & \cdots & 12 \end{bmatrix} \begin{bmatrix} 2256 \\ 2340 \\ \vdots \\ 2328 \end{bmatrix}$$

$$= \begin{bmatrix} 37{,}577 \\ 3{,}429{,}550 \\ 385{,}562 \end{bmatrix}$$

The least squares estimate of $\boldsymbol{\beta}$ is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

or

$$\hat{\boldsymbol{\beta}} = \begin{bmatrix} 14.176004 & -0.129746 & -0.223453 \\ -0.129746 & 1.429184 \times 10^{-3} & -4.763947 \times 10^{-5} \\ -0.223453 & -4.763947 \times 10^{-5} & 2.222381 \times 10^{-2} \end{bmatrix} \begin{bmatrix} 37{,}577 \\ 3{,}429{,}550 \\ 385{,}562 \end{bmatrix}$$

$$= \begin{bmatrix} 1566.07777 \\ 7.62129 \\ 8.58485 \end{bmatrix}$$

Table 10-3 Predicted Values, Residuals, and Other Diagnostics from Example 10-1

Observation i	y_i	Predicted Value $\hat{y}_i$	Residual e_i	h_{ii}	Studentized Residual	D_i	R-Student
1	2256	2244.5	11.5	0.350	0.87	0.137	0.87
2	2340	2352.1	−12.1	0.102	−0.78	0.023	−0.77
3	2426	2414.1	11.9	0.177	0.80	0.046	0.79
4	2293	2294.0	−1.0	0.251	−0.07	0.001	−0.07
5	2330	2346.4	−16.4	0.077	−1.05	0.030	−1.05
6	2368	2389.3	−21.3	0.265	−1.52	0.277	−1.61
7	2250	2252.1	−2.1	0.319	−0.15	0.004	−0.15
8	2409	2383.6	25.4	0.098	1.64	0.097	1.76
9	2364	2385.5	−21.5	0.142	−1.42	0.111	−1.48
10	2379	2369.3	9.7	0.080	0.62	0.011	0.60
11	2440	2416.9	23.1	0.278	1.66	0.354	1.80
12	2364	2384.5	−20.5	0.096	−1.32	0.062	−1.36
13	2404	2396.9	7.1	0.289	0.52	0.036	0.50
14	2317	2316.9	0.1	0.185	0.01	0.000	<0.01
15	2309	2298.8	10.2	0.134	0.67	0.023	0.66
16	2328	2332.1	−4.1	0.156	−0.28	0.005	−0.27

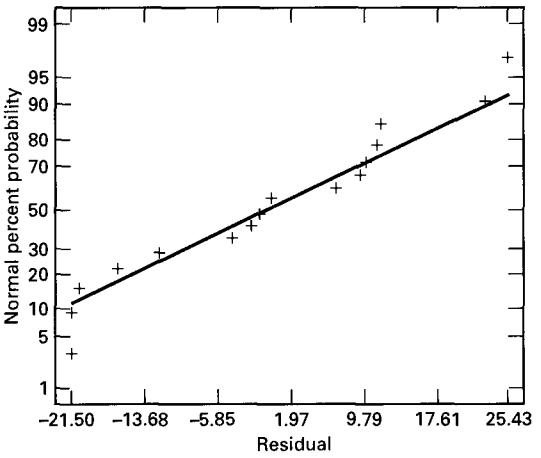


Figure 10-1 Normal probability plot of residuals, Example 10-1.

The least squares fit, with the regression coefficients reported to two decimal places, is

$$\hat{y} = 1566.08 + 7.62x_1 + 8.58x_2$$

The first three columns of Table 10-3 (on the previous page) present the actual observations y_i, the predicted or fitted values $\hat{y}_i$, and the residuals. Figure 10-1 is a normal probability plot of the residuals. Plots of the residuals versus the predicted values $\hat{y}_i$ and versus the two variables x_1 and x_2 are shown in Figures 10-2, 10-3, and 10-4, respectively. Just as in designed experiments, residual plotting is an integral part of regression model building. These plots indicate that there is a tendency for the variance of the observed viscosity to increase with the magnitude of viscosity. Figure 10-3 suggests that the variability in viscosity is increasing as temperature increases.

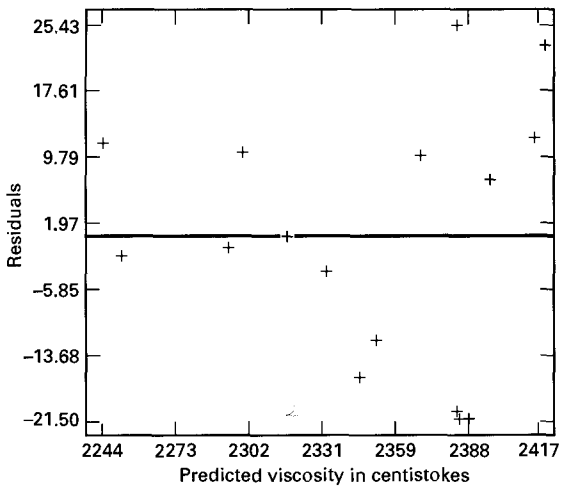


Figure 10-2 Plot of residuals versus predicted viscosity, Example 10-1.

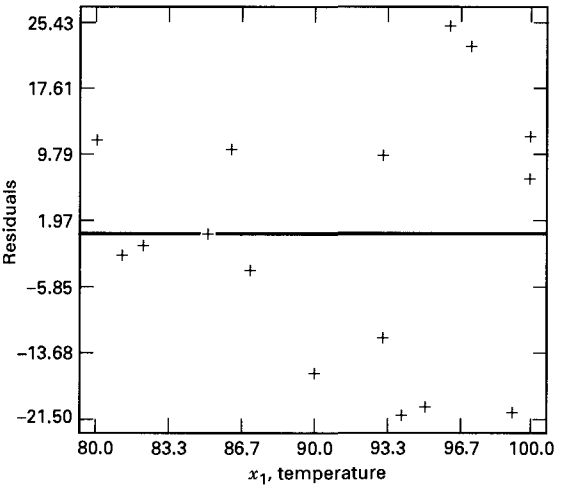


Figure 10-3 Plot of residuals versus x_1 (temperature), Example 10-1.

Using the Computer

Regression model fitting is almost always done using a statistical software package. Table 10-4 (page 402) shows some of the output obtained when Minitab is used to fit the viscosity regression model in Example 10-1. Many of the quantities in this output should be familiar because they have similar meanings to the quantities in the output displays for computer analysis of data from designed experiments. We have seen many such computer outputs previously in the book. In subsequent sections, we will discuss the analysis of variance and t test information in Table 10-4 in detail and will show exactly how these quantities were computed.

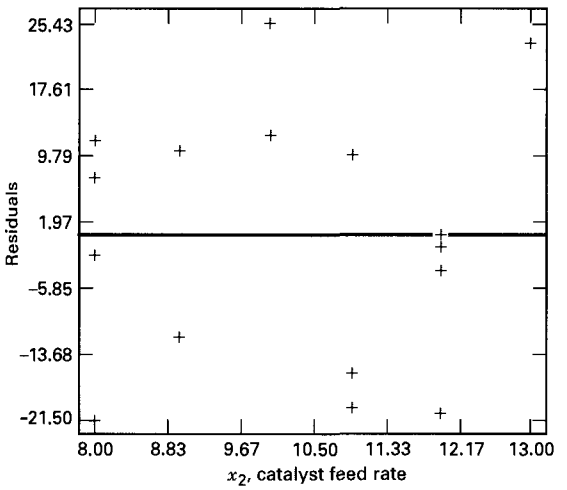
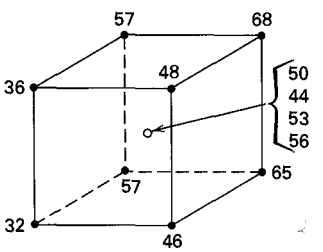


Figure 10-4 Plot of residuals versus x_2 (feed rate), Example 10-1.

Table 10-4 Minitab Output for the Viscosity Regression Model, Example 10-1

Regression Analysis

```
The regression equation is
Viscosity = 1566 + 7.62 Temp + 8.58 Feed Rate

Predictor        Coef      StDev          T          P
Constant      1566.08      61.59      25.43      0.000
Temp           7.6213     0.6184      12.32      0.000
Feed Rat        8.585      2.439       3.52      0.004

S = 16.36       R-Sq = 92.7%     R-Sq(adj) = 91.6%

Analysis of Variance

Source              DF        SS         MS          F          P
Regression           2     44157      22079      82.50      0.000
Residual Error      13      3479        268
Total               15     47636

Source       DF     Seq SS
Temp          1      40841
Feed Rat      1       3316
```



Run	Process Variables: Temp (°C)	Pressure (psig)	Conc. (g/l)	Coded Variables: x_1	x_2	x_3	Yield, y
1	120	40	15	−1	−1	−1	32
2	160	40	15	1	−1	−1	46
3	120	80	15	−1	1	−1	57
4	160	80	15	1	1	−1	65
5	120	40	30	−1	−1	1	36
6	160	40	30	1	−1	1	48
7	120	80	30	−1	1	1	57
8	160	80	30	1	1	1	68
9	140	60	22.5	0	0	0	50
10	140	60	22.5	0	0	0	44
11	140	60	22.5	0	0	0	53
12	140	60	22.5	0	0	0	56

$$x_1 = \frac{\text{Temp} - 140}{20}, \quad x_2 = \frac{\text{Pressure} - 60}{20}, \quad x_3 = \frac{\text{Conc} - 22.5}{7.5}$$

Figure 10-5 Experimental design for Example 10-2.

Fitting Regression Models in Designed Experiments

We have often used a regression model to present the results of a designed experiment in a quantitative form. We now give a complete example showing how this is done. This is followed by three other brief examples that illustrate other useful applications of regression analysis in designed experiments.

EXAMPLE 10-2

Regression Analysis of a 2^3 Factorial Design

A chemical engineer is investigating the yield of a process. Three process variables are of interest: temperature, pressure, and catalyst concentration. Each variable can be run at a low and a high level, and the engineer decides to run a 2^3 design with four center points. The design and the resulting yields are shown in Figure 10-5, where we have shown both the natural levels of the design factor and the $+1, -1$ coded variable notation normally employed in 2^k factorial designs to represent the factor levels.

Suppose that the engineer decides to fit a main effects only model, say

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon$$

For this model the $\mathbf{X}$ matrix and $\mathbf{y}$ vector are

$$\mathbf{X} = \begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 32 \\ 46 \\ 57 \\ 65 \\ 36 \\ 48 \\ 57 \\ 68 \\ 50 \\ 44 \\ 53 \\ 56 \end{bmatrix}$$

It is easy to show that

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} 12 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 8 \end{bmatrix} \qquad \mathbf{X}'\mathbf{y} = \begin{bmatrix} 612 \\ 45 \\ 85 \\ 9 \end{bmatrix}$$

Because $\mathbf{X}'\mathbf{X}$ is *diagonal*, the required inverse is also diagonal, and the least squares estimates of the regression coefficients is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \begin{bmatrix} 1/12 & 0 & 0 & 0 \\ 0 & 1/8 & 0 & 0 \\ 0 & 0 & 1/8 & 0 \\ 0 & 0 & 0 & 1/8 \end{bmatrix} \begin{bmatrix} 612 \\ 45 \\ 85 \\ 9 \end{bmatrix} = \begin{bmatrix} 51.000 \\ 5.625 \\ 10.625 \\ 1.125 \end{bmatrix}$$

The fitted regression model is

$$\hat{y} = 51.000 + 5.625x_1 + 10.625x_2 + 1.125x_3$$

As we have made use of on many occasions, the regression coefficients are closely connected to the effect estimates that would be obtained from the usual analysis of a 2^3 design. For example, the effect of temperature is (refer to Figure 10-5)

$$\begin{aligned} T &= \bar{y}_{T^+} - \bar{y}_{T^-} \\ &= 56.75 - 45.50 \\ &= 11.25 \end{aligned}$$

Notice that the regression coefficient for x_1 is

$$(11.25)/2 = 5.625$$

That is, the regression coefficient is exactly one-half the usual effect estimate. This will always be true for a 2^k design. As noted above, we used this result in Chapters 6 through 8 to produce regression models, fitted values, and residuals for several two-level experiments. This example demonstrates that the effect estimates from a 2^k design are least squares estimates.

In Example 10-2, the inverse matrix is easy to obtain because $\mathbf{X}'\mathbf{X}$ is diagonal. Intuitively, this seems to be advantageous, not only because of the computational simplicity but also because the estimators of all the regression coefficients are uncorrelated; that is, $\text{Cov}(\hat{\beta}_i, \hat{\beta}_j) = 0$. If we can choose the levels of the x variables before the data are collected, we might wish to design the experiment so that a diagonal $\mathbf{X}'\mathbf{X}$ will result.

In practice, it can be relatively easy to do this. We know that the off-diagonal elements in $\mathbf{X}'\mathbf{X}$ are the sums of cross-products of the columns in $\mathbf{X}$. Therefore, we must make the inner product of the columns of $\mathbf{X}$ equal to zero; that is, these columns must be **orthogonal**. Experimental designs that have this property for fitting a regression model are called **orthogonal designs**. In general, the 2^k factorial design is an orthogonal design for fitting the multiple linear regression model.

Regression methods are extremely useful when something "goes wrong" in a designed experiment. This is illustrated in the next two examples.

EXAMPLE 10-3

A 2^3 Factorial Design with a Missing Observation

Consider the 2^3 factorial design with four center points from Example 10-2. Suppose that when this experiment was performed, the run with all variables at the high level (run 8 in Figure 10-5) was missing. This can happen for a variety of reasons; the measurement system can produce a faulty reading, the combination of factor levels may prove infeasible, the experimental unit may be damaged, and so forth.

We will fit the main effects model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon$$

using the 11 remaining observations. The $\mathbf{X}$ matrix and $\mathbf{y}$ vector are

$$\mathbf{X} = \begin{bmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 32 \\ 46 \\ 57 \\ 65 \\ 36 \\ 48 \\ 57 \\ 50 \\ 44 \\ 53 \\ 56 \end{bmatrix}$$

To estimate the model parameters, we form

$$\mathbf{X'X} = \begin{bmatrix} 11 & -1 & -1 & -1 \\ -1 & 7 & -1 & -1 \\ -1 & -1 & 7 & -1 \\ -1 & -1 & -1 & 7 \end{bmatrix} \qquad \mathbf{X'y} = \begin{bmatrix} 544 \\ -23 \\ 17 \\ -59 \end{bmatrix}$$

and then

$$\hat{\boldsymbol{\beta}} = (\mathbf{X'X})^{-1}\mathbf{X'y}$$

$$= \begin{bmatrix} 9.61538 \times 10^{-2} & 1.92307 \times 10^{-2} & 1.92307 \times 10^{-2} & 1.92307 \times 10^{-2} \\ 1.92307 \times 10^{-2} & 0.15385 & 2.88462 \times 10^{-2} & 2.88462 \times 10^{-2} \\ 1.92307 \times 10^{-2} & 2.88462 \times 10^{-2} & 0.15385 & 2.88462 \times 10^{-2} \\ 1.92307 \times 10^{-2} & 2.88462 \times 10^{-2} & 2.88462 \times 10^{-2} & 0.15385 \end{bmatrix} \begin{bmatrix} 544 \\ -23 \\ 17 \\ -59 \end{bmatrix}$$

$$= \begin{bmatrix} 51.25 \\ 5.75 \\ 10.75 \\ 1.25 \end{bmatrix}$$

Therefore, the fitted model is

$$\hat{y} = 51.25 + 5.75x_1 + 10.75x_2 + 1.25x_3$$

Compare this model to the one obtained in Example 10-2, where all 12 observations were used. The regression coefficients are very similar. Because the regression coefficients are closely related to the factor effects, our conclusions would not be seriously affected by the missing observation. However, notice that the effect estimates are no longer orthogonal because $(\mathbf{X'X})$ and its inverse are no longer diagonal.

EXAMPLE 10-4

Inaccurate Levels in Design Factors

When running a designed experiment, it is sometimes difficult to reach and hold the precise factor levels required by the design. Small discrepancies are not important, but large ones are potentially of more concern. Regression methods are useful in the analysis

Table 10-5 Experimental Design for Example 10-4

Run	Process Variables: Temp (°C)	Pressure (psig)	Conc (g/l)	Coded Variables: x_1	x_2	x_3	Yield y
1	125	41	14	−0.75	−0.95	−1.133	32
2	158	40	15	0.90	−1	−1	46
3	121	82	15	−0.95	1.1	−1	57
4	160	80	15	1	1	−1	65
5	118	39	33	−1.10	−1.05	1.14	36
6	163	40	30	1.15	−1	1	48
7	122	80	30	−0.90	1	1	57
8	165	83	30	1.25	1.15	1	68
9	140	60	22.5	0	0	0	50
10	140	60	22.5	0	0	0	44
11	140	60	22.5	0	0	0	53
12	140	60	22.5	0	0	0	56

of a designed experiment where the experimenter has been unable to obtain the required factor levels.

To illustrate, the experiment in Table 10-5 shows a variation of the 2^3 design from Example 10-2, where many of the test combinations are not exactly the ones specified in the design. Most of the difficulty seems to have occurred with the temperature variable.

We will fit the main effects model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon$$

The $\mathbf{X}$ matrix and $\mathbf{y}$ vector are

$$\mathbf{X} = \begin{bmatrix} 1 & -0.75 & -0.95 & -1.133 \\ 1 & 0.90 & -1 & -1 \\ 1 & -0.95 & 1.1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & -1.10 & -1.05 & 1.4 \\ 1 & 1.15 & -1 & 1 \\ 1 & -0.90 & 1 & 1 \\ 1 & 1.25 & 1.15 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 32 \\ 46 \\ 57 \\ 65 \\ 36 \\ 48 \\ 57 \\ 68 \\ 50 \\ 44 \\ 53 \\ 56 \end{bmatrix}$$

To estimate the model parameters, we need

$$\mathbf{X'X} = \begin{bmatrix} 12 & 0.60 & 0.25 & 0.2670 \\ 0.60 & 8.18 & 0.31 & -0.1403 \\ 0.25 & 0.31 & 8.5375 & -0.3437 \\ 0.2670 & -0.1403 & -0.3437 & 9.2437 \end{bmatrix} \qquad \mathbf{X'y} = \begin{bmatrix} 612 \\ 77.55 \\ 161.50 \\ 19.144 \end{bmatrix}$$

Then

$$(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

$$\begin{bmatrix} 8.37447 \times 10^{-2} & -6.09871 \times 10^{-3} & -2.33542 \times 10^{-3} & -2.59833 \times 10^{-3} \\ -6.09871 \times 10^{-3} & 0.12289 & -4.20766 \times 10^{-3} & 1.88490 \times 10^{-3} \\ -2.33542 \times 10^{-3} & -4.20766 \times 10^{-3} & 0.11753 & 4.37851 \times 10^{-3} \\ -2.59833 \times 10^{-3} & 1.88490 \times 10^{-3} & 4.37851 \times 10^{-3} & 0.10845 \end{bmatrix} \begin{bmatrix} 612 \\ 77.5 \\ 161.5 \\ 19.1 \end{bmatrix}$$

$$\begin{bmatrix} 50.36496 \\ 5.41932 \\ 10.16672 \\ 1.07653 \end{bmatrix}$$

The fitted regression model, with the coefficients reported to two decimal places, is

$$\hat{y} = 50.36 + 2x_1 + 10.17x_2 + 1.08x_3$$

Comparing this to the original model in Example 10-2, where the factor levels were exactly those specified by the design, we note very little difference. The practical interpretation of the results of this experiment would not be seriously affected by the inability of the experimenter to achieve the desired factor levels exactly.

EXAMPLE 10-5

De-aliasing Interactions in a Fractional Factorial

We observed in Chapter 8 that it is possible to de-alias interactions in a fractional factorial design by a process called fold over. For a resolution III design, a full fold over is constructed by running a second fraction in which the signs are reversed from those in the original fraction. Then the combined design can be used to de-alias all main effects from the two-factor interactions.

A difficulty with fold over is that it requires a second group of runs of identical size as the original design. It is usually possible to de-alias certain interactions of interest by augmenting the original design with fewer runs than required in a full fold over. Regression methods are an easy way to formulate this problem and see how to solve it.

To illustrate, suppose that we have run a 2_{IV}^{4-1} design. Table 8-3 shows the principal fraction of this design, in which $I = ABCD$. Suppose that after the data from the first eight trials were observed, the largest effects were A, B, C, D (we ignore the three-factor interactions that are aliased with these main effects), and the $AB + CD$ alias chain. The other two alias chains can be ignored, but clearly either AB, or CD, or both two-factor interactions are large. To find out which interactions are important we could, of course, run the alternate fraction, which would require another eight trials. Then all 16 runs could be used to estimate the main effects and the two-factor interactions.

It is possible to de-alias AB and CD in fewer than eight additional trials. Suppose that we wish to fit the model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_{12} x_1 x_2 + \beta_{34} x_3 x_4 + \epsilon$$

where x_1, x_2, x_3, and x_4 are the coded variables representing A, B, C, and D. Using the design in Table 8-3, the $\mathbf{X}$ matrix for this model is

$$\mathbf{X} = \begin{array}{c} \begin{matrix} \quad x_1 & x_2 & x_3 & x_4 & x_1x_2 & x_3x_4 \end{matrix} \\ \begin{bmatrix} 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \end{array}$$

where we have written the variables above the columns to facilitate understanding. Notice that the x_1x_2 column is identical to the x_3x_4 column (as anticipated, because AB or x_1x_2 is aliased with CD or x_3x_4), implying a linear dependency in the columns of $\mathbf{X}$. Therefore we cannot estimate both β_{12} and β_{34} in the model. However, suppose that we add a single run $x_1 = -1$, $x_2 = -1$, $x_3 = -1$, and $x_4 = 1$ from the alternate fraction to the original eight runs. The $\mathbf{X}$ matrix for the model now becomes

$$\mathbf{X} = \begin{array}{c} \begin{matrix} \quad x_1 & x_2 & x_3 & x_4 & x_1x_2 & x_3x_4 \end{matrix} \\ \begin{bmatrix} 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 & -1 \end{bmatrix} \end{array}$$

Notice that the columns x_1x_2 and x_3x_4 are now no longer identical, and we can fit the model including both the x_1x_2 (AB) and x_3x_4 (CD) interactions. The magnitudes of the regression coefficients will give insight regarding which interactions are important.

Although adding a single run will de-alias the AB and CD interactions, this approach does have a disadvantage. Suppose that there is a time effect (or a block effect) between the first eight runs and the last run added above. Add a column to the $\mathbf{X}$ matrix for blocks, and you obtain the following:

$$\mathbf{X} = \begin{array}{c} \begin{matrix} \quad x_1 & x_2 & x_3 & x_4 & x_1x_2 & x_3x_4 & \text{blocks} \end{matrix} \\ \begin{bmatrix} 1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 \end{bmatrix} \end{array}$$

We have assumed the block factor was at the low or "−" level during the first eight runs, and at the high or "+" level during the ninth run. It is easy to see that the sum of the cross-products of every column with the block column does not sum to zero, meaning that blocks are no longer orthogonal to treatments, or that the block effect now affects the estimates of the model regression coefficients. To block orthogonally, you must add an even number of runs. For example, the four runs

x_1	x_2	x_3	x_4
−1	−1	−1	1
1	−1	−1	−1
−1	1	1	1
1	1	1	−1

will de-alias *AB* from *CD* and allow orthogonal blocking (you can see this by writing out the **X** matrix as we did previously).

In general, it is usually straightforward to examine the **X** matrix for the reduced model obtained from a fractional factorial and determine which runs to augment the original design with to de-alias interactions of potential interest. Furthermore, the impact of specific augmentation strategies can be evaluated using the general results for regression models given later in this chapter. There are also computer-based methods for constructing designs that can be useful for **design augmentation** to de-alias effects. We will discuss these **computer-generated designs** in the next chapter.

10-4 HYPOTHESIS TESTING IN MULTIPLE REGRESSION

In multiple linear regression problems, certain tests of hypotheses about the model parameters are helpful in measuring the usefulness of the model. In this section, we describe several important hypothesis-testing procedures. These procedures require that the errors ϵ_i in the model be normally and independently distributed with mean zero and variance σ^2, abbreviated $\epsilon \sim \text{NID}(0, \sigma^2)$. As a result of this assumption, the observations y_i are normally and independently distributed with mean $\beta_0 + \sum_{j=1}^{k} \beta_j x_{ij}$ and variance σ^2.

10-4.1 Test for Significance of Regression

The test for significance of regression is a test to determine if there is a linear relationship between the response variable y and a subset of the regressor variables $x_1, x_2, \ldots, x_k$. The appropriate hypotheses are

$$H_0: \beta_1 = \beta_2 = \cdots = \beta_k = 0$$
$$H_1: \beta_j \neq 0 \quad \text{for at least one } j \tag{10-20}$$

Rejection of H_0 in Equation 10-20 implies that at least one of the regressor variables x_1, $x_2, \ldots, x_k$ contributes significantly to the model. The test procedure involves an analysis

of variance partitioning of the total sum of squares SS_T into a sum of squares due to the model (or to regression) and a sum of squares due to residual (or error), say

$$SS_T = SS_R + SS_E \tag{10-21}$$

Now if the null hypothesis $H_0: \beta_1 = \beta_2 = \cdots = \beta_k = 0$ is true, then SS_R/σ^2 is distributed as χ^2_k, where the number of degrees of freedom for χ^2 are equal to the number of regressor variables in the model. Also, we can show that SS_E/σ^2 is distributed as χ^2_{n-k-1} and that SS_E and SS_R are independent. The test procedure for $H_0: \beta_1 = \beta_2 = \cdots = \beta_k = 0$ is to compute

$$F_0 = \frac{SS_R/k}{SS_E/(n-k-1)} = \frac{MS_R}{MS_E} \tag{10-22}$$

and to reject H_0 if F_0 exceeds $F_{\alpha,k,n-k-1}$. Alternatively, we could use the P-value approach to hypothesis testing and, thus, reject H_0 if the P-value for the statistic F_0 is less than α. The test is usually summarized in an analysis of variance table such as Table 10-6.

A computational formula for SS_R may be found easily. We have derived a computational formula for SS_E in Equation 10-16—that is,

$$SS_E = \mathbf{y}'\mathbf{y} - \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y}$$

Now, because $SS_T = \sum_{i=1}^n y_i^2 - (\sum_{i=1}^n y_i)^2/n = \mathbf{y}'\mathbf{y} - (\sum_{i=1}^n y_i)^2/n$, we may rewrite the foregoing equation as

$$SS_E = \mathbf{y}'\mathbf{y} - \frac{\left(\sum_{i=1}^n y_i\right)^2}{n} - \left[\hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} - \frac{\left(\sum_{i=1}^n y_i\right)^2}{n}\right]$$

or

$$SS_E = SS_T - SS_R$$

Therefore, the regression sum of squares is

$$SS_R = \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} - \frac{\left(\sum_{i=1}^n y_i\right)^2}{n} \tag{10-23}$$

and the error sum of squares is

$$SS_E = \mathbf{y}'\mathbf{y} - \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} \tag{10-24}$$

Table 10-6 Analysis of Variance for Significance of Regression in Multiple Regression

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Regression	SS_R	k	MS_R	MS_R/MS_E
Error or residual	SS_E	$n-k-1$	MS_E	
Total	SS_T	$n-1$		

and the total sum of squares is

$$SS_T = \mathbf{y}'\mathbf{y} - \frac{\left(\sum_{i=1}^{n} y_i\right)^2}{n} \tag{10-25}$$

These computations are almost always performed with regression software. For instance, Table 10-4 shows some of the output from Minitab for the viscosity regression model in Example 10-1. The upper portion in this display is the analysis of variance for the model. The test of significance of regression in this example involves the hypotheses

$$H_0: \beta_1 = \beta_2 = 0$$
$$H_1: \beta_j \neq 0 \qquad \text{for at least one } j$$

The P-value in Table 10-4 for the F statistic (Equation 10-22) is very small, so we would conclude that at least one of the two variables—temperature (x_1) and feed rate (x_2)—has a nonzero regression coefficient.

Table 10-4 also reports the coefficient of multiple determination R^2, where

$$R^2 = \frac{SS_R}{SS_T} = 1 - \frac{SS_E}{SS_T} \tag{10-26}$$

Just as in designed experiments, R^2 is a measure of the amount of reduction in the variability of y obtained by using the regressor variables $x_1, x_2, \ldots, x_k$ in the model. However, as we have noted previously, a large value of R^2 does not necessarily imply that the regression model is a good one. Adding a variable to the model will always increase R^2, regardless of whether the additional variable is statistically significant or not. Thus it is possible for models that have large values of R^2 to yield poor predictions of new observations or estimates of the mean response.

Because R^2 always increases as we add terms to the model, some regression model builders prefer to use an **adjusted R^2 statistic** defined as

$$R^2_{\text{adj}} = 1 - \frac{SS_E/(n-p)}{SS_T/(n-1)} = 1 - \left(\frac{n-1}{n-p}\right)(1 - R^2) \tag{10-27}$$

In general, the adjusted R^2 statistic will not always increase as variables are added to the model. In fact, if unnecessary terms are added, the value of R^2_{adj} will often decrease.

For example, consider the viscosity regression model. The adjusted R^2 for the model is shown in Table 10-4. It is computed as

$$\begin{aligned} R^2_{\text{adj}} &= 1 - \left(\frac{n-1}{n-p}\right)(1 - R^2) \\ &= 1 - \left(\frac{15}{13}\right)(1 - 0.92697) \\ &= 0.915735 \end{aligned}$$

which is very close to the ordinary R^2. When R^2 and R^2_{adj} differ dramatically, there is a good chance that nonsignificant terms have been included in the model.

10-4.2 Tests on Individual Regression Coefficients and Groups of Coefficients

We are frequently interested in testing hypotheses on the individual regression coefficients. Such tests would be useful in determining the value of each of the regressor variables in the regression model. For example, the model might be more effective with the inclusion of additional variables or perhaps with the deletion of one or more of the variables already in the model.

Adding a variable to the regression model always causes the sum of squares for regression to increase and the error sum of squares to decrease. We must decide whether the increase in the regression sum of squares is sufficient to warrant using the additional variable in the model. Furthermore, adding an unimportant variable to the model can actually increase the mean square error, thereby decreasing the usefulness of the model.

The hypotheses for testing the significance of any individual regression coefficient, say β_j, are

$$H_0: \beta_j = 0$$
$$H_1: \beta_j \neq 0$$

If $H_0: \beta_j = 0$ is not rejected, then this indicates that x_j can be deleted from the model. The test statistic for this hypothesis is

$$t_0 = \frac{\hat{\beta}_j}{\sqrt{\hat{\sigma}^2 C_{jj}}} \tag{10-28}$$

where C_{jj} is the diagonal element of $(\mathbf{X}'\mathbf{X})^{-1}$ corresponding to $\hat{\beta}_j$. The null hypothesis $H_0: \beta_j = 0$ is rejected if $|t_0| > t_{\alpha/2,n-k-1}$. Note that this is really a partial or marginal test, because the regression coefficient $\hat{\beta}_j$ depends on all the other regressor variables x_i $(i \neq j)$ that are in the model.

The denominator of Equation 10-28, $\sqrt{\hat{\sigma}^2 C_{jj}}$, is often called the **standard error** of the regression coefficient $\hat{\beta}_j$. That is,

$$se(\hat{\beta}_j) = \sqrt{\hat{\sigma}^2 C_{jj}} \tag{10-29}$$

Therefore, an equivalent way to write the test statistic in Equation (10-28) is

$$t_0 = \frac{\hat{\beta}_j}{se(\hat{\beta}_j)} \tag{10-30}$$

Most regression computer programs provide the t test for each model parameter. For example, consider Table 10-4, which contains the Minitab output for Example 10-1. The upper portion of this table gives the least squares estimate of each parameter, the standard error, the t statistic, and the corresponding P-value. We would conclude that both variables, temperature and feed rate, contribute significantly to the model.

We may also directly examine the contribution to the regression sum of squares for a particular variable, say x_j, given that other variables x_i $(i \neq j)$ are included in the model. The procedure for doing this is the general regression significance test or, as it is often called, the **extra sum of squares method**. This procedure can also be used to investigate the contribution of a *subset* of the regressor variables to the model. Consider the regression model with k regressor variables:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where $\mathbf{y}$ is $(n \times 1)$, $\mathbf{X}$ is $(n \times p)$, $\boldsymbol{\beta}$ is $(p \times 1)$, $\boldsymbol{\epsilon}$ is $(n \times 1)$, and $p = k + 1$. We would like to determine if the subset of regressor variables $x_1, x_2, \ldots, x_r$ $(r < k)$ contribute significantly to the regression model. Let the vector of regression coefficients be partitioned as follows:

$$\boldsymbol{\beta} = \begin{bmatrix} \boldsymbol{\beta}_1 \\ \boldsymbol{\beta}_2 \end{bmatrix}$$

where $\boldsymbol{\beta}_1$ is $(r \times 1)$ and $\boldsymbol{\beta}_2$ is $[(p - r) \times 1]$. We wish to test the hypotheses

$$\begin{aligned} H_0&: \boldsymbol{\beta}_1 = \mathbf{0} \\ H_1&: \boldsymbol{\beta}_1 \neq \mathbf{0} \end{aligned} \tag{10-31}$$

The model may be written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\epsilon} \tag{10-32}$$

where $\mathbf{X}_1$ represents the columns of $\mathbf{X}$ associated with $\boldsymbol{\beta}_1$ and $\mathbf{X}_2$ represents the columns of $\mathbf{X}$ associated with $\boldsymbol{\beta}_2$.

For the **full model** (including both $\boldsymbol{\beta}_1$ and $\boldsymbol{\beta}_2$), we know that $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$. Also, the regression sum of squares for all variables including the intercept is

$$SS_R(\boldsymbol{\beta}) = \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} \qquad (p \text{ degrees of freedom})$$

and

$$MS_E = \frac{\mathbf{y}'\mathbf{y} - \hat{\boldsymbol{\beta}}\mathbf{X}'\mathbf{y}}{n - p}$$

$SS_R(\boldsymbol{\beta})$ is called the regression sum of squares due to $\boldsymbol{\beta}$. To find the contribution of the terms in $\boldsymbol{\beta}_1$ to the regression, we fit the model assuming the null hypothesis $H_0: \boldsymbol{\beta}_1 = \mathbf{0}$ to be true. The **reduced model** is found from Equation 10-32 with $\boldsymbol{\beta}_1 = \mathbf{0}$:

$$\mathbf{y} = \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\epsilon} \tag{10-33}$$

The least squares estimator of $\boldsymbol{\beta}_2$ is $\hat{\boldsymbol{\beta}}_2 = (\mathbf{X}_2'\mathbf{X}_2)^{-1}\mathbf{X}_2'\mathbf{y}$, and

$$SS_R(\boldsymbol{\beta}_2) = \hat{\boldsymbol{\beta}}_2'\mathbf{X}_2'\mathbf{y} \qquad (p - r \text{ degrees of freedom}) \tag{10-34}$$

The regression sum of squares due to $\boldsymbol{\beta}_1$ given that $\boldsymbol{\beta}_2$ is already in the model is

$$SS_R(\boldsymbol{\beta}_1 \mid \boldsymbol{\beta}_2) = SS_R(\boldsymbol{\beta}) - SS_R(\boldsymbol{\beta}_2) \tag{10-35}$$

This sum of squares has r degrees of freedom. It is the "extra sum of squares" due to $\boldsymbol{\beta}_1$. Note that $SS_R(\boldsymbol{\beta}_1 \mid \boldsymbol{\beta}_2)$ is the increase in the regression sum of squares due to including the variables $x_1, x_2, \ldots, x_r$ in the model.

Now, $SS_R(\boldsymbol{\beta}_1 \mid \boldsymbol{\beta}_2)$ is independent of MS_E, and the null hypothesis $\boldsymbol{\beta}_1 = \mathbf{0}$ may be tested by the statistic

$$F_0 = \frac{SS_R(\boldsymbol{\beta}_1 \mid \boldsymbol{\beta}_2)/r}{MS_E} \tag{10-36}$$

If $F_0 > F_{\alpha,r,n-p}$, we reject H_0, concluding that at least one of the parameters in $\boldsymbol{\beta}_1$ is not zero and, consequently, at least one of the variables $x_1, x_2, \ldots, x_r$ in $\mathbf{X}_1$ contributes significantly to the regression model. Some authors call the test in Equation 10-36 a **partial F test.**

The partial F test is very useful. We can use it to measure the contribution of x_j as if it were the last variable added to the model by computing

$$SS_R(\beta_j | \beta_0, \beta_1, \ldots, \beta_{j-1}, \beta_{j+1}, \ldots, \beta_k)$$

This is the increase in the regression sum of squares due to adding x_j to a model that already includes $x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_k$. Note that the partial F test on a single variable x_j is equivalent to the t test in Equation 10-28. However, the partial F test is a more general procedure in that we can measure the effect of sets of variables.

EXAMPLE 10-6

Consider the viscosity data in Example 10-1. Suppose that we wish to investigate the contribution of the variable x_2 (feed rate) to the model. That is, the hypotheses we wish to test are

$$H_0: \beta_2 = 0$$
$$H_1: \beta_2 \neq 0$$

This will require the extra sum of squares due to β_2, or

$$\begin{aligned} SS_R(\beta_2 | \beta_1, \beta_0) &= SS_R(\beta_0, \beta_1, \beta_2) - SS_R(\beta_0, \beta_1) \\ &= SS_R(\beta_1, \beta_2 | \beta_0) - SS_R(\beta_2 | \beta_0) \end{aligned}$$

Now from Table 10-4, where we tested for significance of regression, we have

$$SS_R(\beta_1, \beta_2 | \beta_0) = 44{,}157.1$$

which was called the model sum of squares in the table. This sum of squares has two degrees of freedom.

The reduced model is

$$y = \beta_0 + \beta_1 x_1 + \epsilon$$

The least squares fit for this model is

$$\hat{y} = 1652.3955 + 7.6397 x_1$$

and the regression sum of squares for this model (with one degree of freedom) is

$$SS_R(\beta_1 | \beta_0) = 40{,}840.8$$

Note that $SS_R(\beta_1 | \beta_0)$ is shown at the bottom of the Minitab output in Table 10-4 under the heading "Seq SS." Therefore,

$$\begin{aligned} SS_R(\beta_2 | \beta_0, \beta_1) &= 44{,}157.1 - 40{,}840.8 \\ &= 3316.3 \end{aligned}$$

with $2 - 1 = 1$ degree of freedom. This is the increase in the regression sum of squares that results from adding x_2 to a model already containing x_1, and it is shown at the bottom of the Minitab output on Table 10-4. To test $H_0: \beta_2 = 0$, from the test statistic we obtain

$$F_0 = \frac{SS_R(\beta_2 | \beta_0, \beta_1)/1}{MS_E} = \frac{3316.3/1}{267.604} = 12.3926$$

Note that MS_E from the full model (Table 10-4) is used in the denominator of F_0. Now, because $F_{0.05,1,13} = 1.67$, we would reject $H_0: \beta_2 = 0$ and conclude that x_2 (feed rate) contributes significantly to the model.

Because this partial F test involves only a single regressor, it is equivalent to the t test because the square of a t random variable with ν degrees of freedom is an F random variable with 1 and ν degrees of freedom. To see this, note from Table 10-4 that the t statistic for $H_0: \beta_2 = 0$ resulted in $t_0 = 3.5203$ and that $t_0^2 = (3.5203)^2 = 12.3925 \simeq F_0$.

10-5 CONFIDENCE INTERVALS IN MULTIPLE REGRESSION

It is often necessary to construct confidence interval estimates for the regression coefficients $\{\beta_j\}$ and for other quantities of interest from the regression model. The development of a procedure for obtaining these confidence intervals requires that we assume the errors $\{\epsilon_i\}$ to be normally and independently distributed with mean zero and variance σ^2, the same assumption made in the section on hypothesis testing in Section 10-4.

10-5.1 Confidence Intervals on the Individual Regression Coefficients

Because the least squares estimator $\hat{\boldsymbol{\beta}}$ is a linear combination of the observations, it follows that $\hat{\boldsymbol{\beta}}$ is normally distributed with mean vector $\boldsymbol{\beta}$ and covariance matrix $\sigma^2(\mathbf{X}'\mathbf{X})^{-1}$. Then each of the statistics

$$\frac{\hat{\beta}_j - \beta_j}{\sqrt{\hat{\sigma}^2 C_{jj}}} \qquad j = 0, 1, \ldots, k \tag{10-37}$$

is distributed as t with $n - p$ degrees of freedom, where C_{jj} is the (jj)th element of the $(\mathbf{X}'\mathbf{X})^{-1}$ matrix, and $\hat{\sigma}^2$ is the estimate of the error variance, obtained from Equation 10-17. Therefore, a $100(1 - \alpha)$ percent confidence interval for the regression coefficient β_j, $j = 0, 1, \ldots, k$, is

$$\hat{\beta}_j - t_{\alpha/2,n-p}\sqrt{\hat{\sigma}^2 C_{jj}} \leq \beta_j \leq \hat{\beta}_j + t_{\alpha/2,n-p}\sqrt{\hat{\sigma}^2 C_{jj}} \tag{10-38}$$

Note that this confidence interval could also be written as

$$\hat{\beta}_j - t_{\alpha/2,n-p} se(\hat{\beta}_j) \leq \beta_j \leq \hat{\beta}_j + t_{\alpha/2,n-p} se(\hat{\beta}_j)$$

because $se(\hat{\beta}_j) = \sqrt{\hat{\sigma}^2 C_{jj}}$.

EXAMPLE 10-7

We will construct a 95 percent confidence interval for the parameter β_1 in Example 10-1. Now $\hat{\beta}_1 = 7.62129$, and because $\hat{\sigma}^2 = 267.604$ and $C_{11} = 1.429184 \times 10^{-3}$, we find that

$$\hat{\beta}_1 - t_{0.025,13}\sqrt{\hat{\sigma}^2 C_{11}} \leq \beta_1 \leq \hat{\beta}_1 + t_{0.025,13}\sqrt{\hat{\sigma}^2 C_{11}}$$

$$7.62129 - 2.16\sqrt{(267.604)(1.429184 \times 10^{-3})} \leq \beta_1 \leq 7.62129 + 2.16\sqrt{(267.604)(1.429184 \times 10^{-3})}$$

$$7.62129 - 2.16(0.6184) \leq \beta_1 \leq 7.62129 + 2.16(0.6184)$$

and the 95 percent confidence interval on β_1 is

$$6.2855 \leq \beta_1 \leq 8.9570$$

10-5.2 Confidence Interval on the Mean Response

We may also obtain a confidence interval on the mean response at a particular point, say, $x_{01}, x_{02}, \ldots, x_{0k}$. We first define the vector

$$\mathbf{x}_0 = \begin{bmatrix} 1 \\ x_{01} \\ x_{02} \\ \vdots \\ x_{0k} \end{bmatrix}$$

The mean response at this point is

$$\mu_{y|\mathbf{x}_0} = \beta_0 + \beta_1 x_{01} + \beta_2 x_{02} + \cdots + \beta_k x_{0k} = \mathbf{x}_0'\boldsymbol{\beta}$$

The estimated mean response at this point is

$$\hat{y}(\mathbf{x}_0) = \mathbf{x}_0'\hat{\boldsymbol{\beta}} \tag{10-39}$$

This estimator is unbiased, because $E[\hat{y}(\mathbf{x}_0)] = E(\mathbf{x}_0'\hat{\boldsymbol{\beta}}) = \mathbf{x}_0'\boldsymbol{\beta} = \mu_{y|\mathbf{x}_0}$, and the variance of $\hat{y}(\mathbf{x}_0)$ is

$$V[\hat{y}(\mathbf{x}_0)] = \sigma^2\mathbf{x}_0'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_0 \tag{10-40}$$

Therefore, a $100(1 - \alpha)$ percent confidence interval on the mean response at the point $x_{01}, x_{02}, \ldots, x_{0k}$ is

$$\hat{y}(\mathbf{x}_0) - t_{\alpha/2,n-p}\sqrt{\hat{\sigma}^2\mathbf{x}_0'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_0} \leq \mu_{y|\mathbf{x}_0} \leq \hat{y}(\mathbf{x}_0) + t_{\alpha/2,n-p}\sqrt{\hat{\sigma}^2\mathbf{x}_0'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_0} \tag{10-41}$$

10-6 PREDICTION OF NEW RESPONSE OBSERVATIONS

A regression model can be used to predict future observations on the response y corresponding to particular values of the regressor variables, say $x_{01}, x_{02}, \ldots, x_{0k}$. If $\mathbf{x}_0' = [1, x_{01}, x_{02}, \ldots, x_{0k}]$, then a point estimate for the future observation y_0 at the point $x_{01}, x_{02}, \ldots, x_{0k}$ is computed from Equation 10-39:

$$\hat{y}(\mathbf{x}_0) = \mathbf{x}_0'\hat{\boldsymbol{\beta}}$$

A $100(1 - \alpha)$ percent **prediction interval** for this future observation is

$$\hat{y}(\mathbf{x}_0) - t_{\alpha/2,n-p}\sqrt{\hat{\sigma}^2(1 + \mathbf{x}_0'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_0)} \leq y_0 \leq \hat{y}(\mathbf{x}_0) + t_{\alpha/2,n-p}\sqrt{\hat{\sigma}^2(1 + \mathbf{x}_0'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_0)} \tag{10-42}$$

In predicting new observations and in estimating the mean response at a given point $x_{01}, x_{02}, \ldots, x_{0k}$, we must be careful about extrapolating beyond the region containing the original observations. It is very possible that a model that fits well in the region of the original data will no longer fit well outside of that region.

10-7 REGRESSION MODEL DIAGNOSTICS

As we emphasized in designed experiments, **model adequacy checking** is an important part of the data analysis procedure. This is equally important in building regression models, and as we illustrated in Example 10-1, the **residual plots** that we used with

designed experiments should always be examined for a regression model. In general, it is always necessary to (1) examine the fitted model to ensure that it provides an adequate approximation to the true system and (2) verify that none of the least squares regression assumptions are violated. The regression model will probably give poor or misleading results unless it is an adequate fit.

In addition to residual plots, there are other model diagnostics that are frequently useful in regression. This section briefly summarizes some of these procedures. For more complete presentations, see Montgomery and Peck (1992) and Myers (1990).

10-7.1 Scaled Residuals and PRESS

Standardized and Studentized Residuals

Many model builders prefer to work with **scaled residuals** in contrast to the ordinary least squares residuals. These scaled residuals often convey more information than do the ordinary residuals.

One type of scaled residual is the **standardized residual**:

$$d_i = \frac{e_i}{\hat{\sigma}} \qquad i = 1, 2, \ldots, n \tag{10-43}$$

where we generally use $\hat{\sigma} = \sqrt{MS_E}$ in the computation. These standardized residuals have mean zero and approximately unit variance; consequently, they are useful in looking for **outliers**. Most of the standardized residuals should lie in the interval $-3 \leq d_i \leq 3$, and any observation with a standardized residual outside of this interval is potentially unusual with respect to its observed response. These outliers should be carefully examined, because they may represent something as simple as a data-recording error or something of more serious concern, such as a region of the regressor variable space where the fitted model is a poor approximation to the true response surface.

The standardizing process in Equation (10-43) scales the residuals by dividing them by their approximate average standard deviation. In some data sets, residuals may have standard deviations that differ greatly. We now present a scaling that takes this into account.

The vector of fitted values $\hat{y}_i$ corresponding to the observed values y_i is

$$\begin{aligned} \hat{\mathbf{y}} &= \mathbf{X}\hat{\boldsymbol{\beta}} \\ &= \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} \\ &= \mathbf{H}\mathbf{y} \end{aligned} \tag{10-44}$$

The $n \times n$ matrix $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ is usually called the "hat" matrix because it maps the vector of observed values into a vector of fitted values. The hat matrix and its properties play a central role in regression analysis.

The residuals from the fitted model may be conveniently written in matrix notation as

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}}$$

and it turns out that the covariance matrix of the residuals is

$$\text{Cov}(\mathbf{e}) = \sigma^2(\mathbf{I} - \mathbf{H}) \tag{10-45}$$

The matrix $\mathbf{I} - \mathbf{H}$ is generally not diagonal, so the residuals have different variances and they are correlated.

Thus, the variance of the ith residual is

$$V(e_i) = \sigma^2(1 - h_{ii}) \tag{10-46}$$

where h_{ii} is the ith diagonal element of $\mathbf{H}$. Because $0 \leq h_{ii} \leq 1$, using the residual mean square MS_E to estimate the variance of the residuals actually overestimates $V(e_i)$. Furthermore, because h_{ii} is a measure of the location of the ith point in x-space, the variance of e_i depends on where the point x_i lies. Generally, residuals near the center of the x space have larger variance than do residuals at more remote locations. Violations of model assumptions are more likely at remote points, and these violations may be hard to detect from inspection of e_i (or d_i) because their residuals will usually be smaller.

We recommend taking this inequality of variance into account when scaling the residuals. We suggest plotting the **studentized residuals**:

$$r_i = \frac{e_i}{\sqrt{\hat{\sigma}^2(1 - h_{ii})}} \qquad i = 1, 2, \ldots, n \tag{10-47}$$

with $\hat{\sigma}^2 = MS_E$ instead of e_i (or d_i). The studentized residuals have constant variance $V(r_i) = 1$ regardless of the location of $\mathbf{x}_i$ when the form of the model is correct. In many situations the variance of the residuals stabilizes, particularly for large data sets. In these cases there may be little difference between the standardized and studentized residuals. Thus standardized and studentized residuals often convey equivalent information. However, because any point with a large residual and a large h_{ii} is potentially highly influential on the least squares fit, examination of the studentized residuals is generally recommended. Table 10-3 displays the hat diagonals h_{ii} and the studentized residuals for the viscosity regression model in Example 10-1.

PRESS Residuals

The prediction error sum of squares (PRESS) provides a useful residual scaling. To calculate PRESS, we select an observation—for example, i. We fit the regression model to the remaining $n - 1$ observations and use this equation to predict the withheld observation y_i. Denoting this predicted value $\hat{y}_{(i)}$, we may find the prediction error for point i as $e_{(i)} = y_i - \hat{y}_{(i)}$. The prediction error is often called the ith PRESS residual. This procedure is repeated for each observation $i = 1, 2, \ldots, n$, producing a set of n PRESS residuals $e_{(1)}, e_{(2)}, \ldots, e_{(n)}$. Then the PRESS statistic is defined as the sum of squares of the n PRESS residuals as in

$$\text{PRESS} = \sum_{i=1}^{n} e_{(i)}^2 = \sum_{i=1}^{n} [y_i - \hat{y}_{(i)}]^2 \tag{10-48}$$

Thus PRESS uses each possible subset of $n - 1$ observations as an estimation data set, and every observation in turn is used to form a prediction data set.

It would initially seem that calculating PRESS requires fitting n different regressions. However, it is possible to calculate PRESS from the results of a single least squares fit to all n observations. It turns out that the ith PRESS residual is

$$e_{(i)} = \frac{e_i}{1 - h_{ii}} \tag{10-49}$$

Thus because PRESS is just the sum of the squares of the PRESS residuals, a simple computing formula is

$$\text{PRESS} = \sum_{i=1}^{n} \left(\frac{e_i}{1 - h_{ii}}\right)^2 \tag{10-50}$$

From Equation 10-49 it is easy to see that the PRESS residual is just the ordinary residual weighted according to the diagonal elements of the hat matrix h_{ii}. Data points for which h_{ii} are large will have large PRESS residuals. These observations will generally be **high influence** points. Generally, a large difference between the ordinary residual and the PRESS residuals will indicate a point where the model fits the data well, but a model built without that point predicts poorly. In the next section we will discuss some other measures of influence.

Finally, we note that PRESS can be used to compute an approximate R^2 for prediction, say

$$R^2_{\text{Prediction}} = 1 - \frac{\text{PRESS}}{S_{yy}} \tag{10-51}$$

This statistic gives some indication of the predictive capability of the regression model. For the viscosity regression model from Example 10-1, we can compute the PRESS residuals using the ordinary residuals and the values of h_{ii} found in Table 10-3. The corresponding value of the PRESS statistic is PRESS = 5207.7. Then

$$\begin{aligned} R^2_{\text{Prediction}} &= 1 - \frac{\text{PRESS}}{S_{yy}} \\ &= 1 - \frac{5207.7}{47{,}635.9} \\ &= 0.8907 \end{aligned}$$

Therefore we could expect this model to "explain" about 89 percent of the variability in predicting new observations, as compared to the approximately 93 percent of the variability in the original data explained by the least squares fit. The overall predictive capability of the model based on this criterion seems very satisfactory.

R-Student

The studentized residual r_i discussed above is often considered an outlier diagnostic. It is customary to use MS_E as an estimate of σ^2 in computing r_i. This is referred to as internal scaling of the residual because MS_E is an internally generated estimate of σ^2 obtained from fitting the model to all n observations. Another approach would be to use an estimate of σ^2 based on a data set with the ith observation removed. We denote the estimate of σ^2 so obtained by $S^2_{(i)}$. We can show that

$$S^2_{(i)} = \frac{(n-p)MS_E - e_i^2/(1-h_{ii})}{n-p-1} \tag{10-52}$$

The estimate of σ^2 in Equation 10-52 is used instead of MS_E to produce an externally studentized residual, usually called R-student, given by

$$t_i = \frac{e_i}{\sqrt{S^2_{(i)}(1-h_{ii})}} \qquad i = 1, 2, \ldots, n \tag{10-53}$$

In many situations, t_i will differ little from the studentized residual r_i. However, if the ith observation is influential, then $S^2_{(i)}$ can differ significantly from MS_E, and thus the R-student will be more sensitive to this point. Furthermore, under the standard assumptions, t_i has a t_{n-p-1} distribution. Thus R-student offers a more formal procedure for outlier detection via hypothesis testing. Table 10-3 displays the values of R-student for the viscosity regression model in Example 10-1. None of those values is unusually large.

10-7.2 Influence Diagnostics

We occasionally find that a small subset of the data exerts a disproportionate influence on the fitted regression model. That is, parameter estimates or predictions may depend more on the influential subset than on the majority of the data. We would like to locate these influential points and assess their impact on the model. If these influential points are "bad" values, they should be eliminated. On the other hand, there may be nothing wrong with these points. But if they control key model properties, we would like to know it, because it could affect the use of the model. In this section we describe and illustrate some useful measures of influence.

Leverage Points

The disposition of points in x space is important in determining model properties. In particular, remote observations potentially have disproportionate leverage on the parameter estimates, predicted values, and the usual summary statistics.

The hat matrix $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ is very useful in identifying influential observations. As noted earlier, $\mathbf{H}$ determines the variances and covariances of $\hat{\mathbf{y}}$ and $\mathbf{e}$, because $V(\hat{\mathbf{y}}) = \sigma^2\mathbf{H}$ and $V(\mathbf{e}) = \sigma^2(\mathbf{I} - \mathbf{H})$. The elements h_{ij} of $\mathbf{H}$ may be interpreted as the amount of leverage exerted by y_j on $\hat{y}_i$. Thus, inspection of the elements of $\mathbf{H}$ can reveal points that are potentially influential by virtue of their location in x space. Attention is usually focused on the diagonal elements h_{ii}. Because $\sum_{i=1}^{n} h_{ii} = \text{rank}(\mathbf{H}) = \text{rank}(\mathbf{X}) = p$, the average size of the diagonal element of the $\mathbf{H}$ matrix is p/n. As a rough guideline, then, if a diagonal element h_{ii} is greater than $2p/n$, observation i is a high-leverage point. To apply this to the viscosity model in Example 10-1, note that $2p/n = 2(3)/16 = 0.375$. Table 10-3 gives the hat diagonals h_{ii} for the first-order model; because none of the h_{ii} exceeds 0.375, we would conclude that there are no leverage points in these data.

Influence on Regression Coefficients

The hat diagonals will identify points that are potentially influential due to their location in x space. It is desirable to consider both the location of the point and the response variable in measuring influence. Cook (1977, 1979) has suggested using a measure of the squared distance between the least squares estimate based on all n points $\hat{\boldsymbol{\beta}}$ and the estimate obtained by deleting the i point, say $\hat{\boldsymbol{\beta}}_{(i)}$. This distance measure can be expressed as

$$D_i = \frac{(\hat{\boldsymbol{\beta}}_{(i)} - \hat{\boldsymbol{\beta}})'\mathbf{X}'\mathbf{X}(\hat{\boldsymbol{\beta}}_{(i)} - \hat{\boldsymbol{\beta}})}{pMS_E} \qquad i = 1, 2, \ldots, n \tag{10-54}$$

A reasonable cutoff for D_i is unity. That is, we usually consider observations for which $D_i > 1$ to be influential.

The D_i statistic is actually calculated from

$$D_i = \frac{r_i^2}{p}\frac{V[\hat{y}(x_i)]}{V(e_i)} = \frac{r_i^2}{p}\frac{h_{ii}}{(1 - h_{ii})} \qquad i = 1, 2, \ldots, n \tag{10-55}$$

Note that, apart from the constant p, D_i is the product of the square of the ith studentized residual and $h_{ii}/(1 - h_{ii})$. This ratio can be shown to be the distance from the vector $\mathbf{x}_i$ to the centroid of the remaining data. Thus, D_i is made up of a component that reflects how well the model fits the ith observation y_i and a component that measures how far

that point is from the rest of the data. Either component (or both) may contribute to a large value of D_i.

Table 10-3 presents the values of D_i for the regression model fit to the viscosity data in Example 10-1. None of these values of D_i exceeds 1, so there is no strong evidence of influential observations in these data.

10-8 TESTING FOR LACK OF FIT

In Section 6-6 we showed how adding center points to a 2^k factorial design allows the experimenter to obtain an estimate of pure experimental error. This allows the partitioning of the residual sum of squares SS_E into two components; that is

$$SS_E = SS_{PE} + SS_{LOF}$$

where SS_{PE} is the sum of squares due to pure error and SS_{LOF} is the sum of squares due to lack of fit.

We may give a general development of this partitioning in the context of a regression model. Suppose that we have n_i observations on the response at the ith level of the regressors $\mathbf{x}_i$, $i = 1, 2, \ldots, m$. Let y_{ij} denote the jth observation on the response at $\mathbf{x}_i$, $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n_i$. There are $n = \sum_{i=1}^{m} n_i$ total observations. We may write the (ij)th residual as

$$y_{ij} - \hat{y}_i = (y_{ij} - \bar{y}_i) + (\bar{y}_i - \hat{y}_i) \tag{10-56}$$

where $\bar{y}_i$ is the average of the n_i observations at $\mathbf{x}_i$. Squaring both sides of Equation 10-56 and summing over i and j yields

$$\sum_{i=1}^{m}\sum_{j=1}^{n_i} (y_{ij} - \hat{y}_i)^2 = \sum_{i=1}^{m}\sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 + \sum_{i=1}^{m} n_i(\bar{y}_i - \hat{y}_i)^2 \tag{10-57}$$

The left-hand side of Equation 10-57 is the usual residual sum of squares. The two components on the right-hand side measure pure error and lack of fit. We see that the pure error sum of squares

$$SS_{PE} = \sum_{i=1}^{m}\sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 \tag{10-58}$$

is obtained by computing the corrected sum of squares of the repeat observations at each level of $\mathbf{x}$ and then pooling over the m levels of $\mathbf{x}$. If the assumption of constant variance is satisfied, this is a **model-independent** measure of pure error because only the variability of the y's at each $\mathbf{x}_i$ level is used to compute SS_{PE}. Because there are $n_i - 1$ degrees of freedom for pure error at each level $\mathbf{x}_i$, the total number of degrees of freedom associated with the pure error sum of squares is

$$\sum_{i=1}^{m} (n_i - 1) = n - m \tag{10-59}$$

The sum of squares for lack of fit

$$SS_{LOF} = \sum_{i=1}^{m} n_i(\bar{y}_i - \hat{y}_i)^2 \tag{10-60}$$

is a weighted sum of squared deviations between the mean response $\bar{y}_i$ at each $\mathbf{x}_i$ level and the corresponding fitted value. If the fitted values $\hat{y}_i$ are close to the corresponding average responses $\bar{y}_i$, then there is a strong indication that the regression function is linear. If the $\hat{y}_i$ deviate greatly from the $\bar{y}_i$, then it is likely that the regression function is not linear. There are $m - p$ degrees of freedom associated with SS_{LOF} because there are m levels of $\mathbf{x}$, and p degrees of freedom are lost because p parameters must be estimated for the model. Computationally we usually obtain SS_{LOF} by subtracting SS_{PE} from SS_E.

The test statistic for lack of fit is

$$F_0 = \frac{SS_{LOF}/(m - p)}{SS_{PE}/(n - m)} = \frac{MS_{LOF}}{MS_{PE}} \tag{10-61}$$

The expected value of MS_{PE} is σ^2, and the expected value of MS_{LOF} is

$$E(MS_{LOF}) = \sigma^2 + \frac{\sum_{i=1}^{m} n_i \left[E(y_i) - \beta_0 - \sum_{j=1}^{k} \beta_j x_{ij} \right]^2}{m - 2} \tag{10-62}$$

If the true regression function is linear, then $E(y_i) = \beta_0 + \sum_{j=1}^{k} \beta_j x_{ij}$, and the second term of Equation 10-62 is zero, resulting in $E(MS_{LOF}) = \sigma^2$. However, if the true regression function is not linear, then $E(y_i) \neq \beta_0 + \sum_{j=1}^{k} \beta_j x_{ij}$, and $E(MS_{LOF}) > \sigma^2$. Furthermore, if the true regression function is linear, then the statistic F_0 follows the $F_{m-p,n-m}$ distribution. Therefore, to test for lack of fit, we would compute the test statistic F_0 and conclude that the regression function is not linear if $F_0 > F_{\alpha,m-p,n-m}$.

This test procedure may be easily incorporated into the analysis of variance. If we conclude that the regression function is not linear, then the tentative model must be abandoned and attempts made to find a more appropriate equation. Alternatively, if F_0 does not exceed $F_{\alpha,m-p,n-m}$, there is no strong evidence of lack of fit and MS_{PE} and MS_{LOF} are often combined to estimate σ^2. Example 6-6 is a very complete illustration of this procedure, where the replicate runs are center points in a 2^2 factorial design.

10-9 PROBLEMS

10-1. The tensile strength of a paper product is related to the amount of hardwood in the pulp. Ten samples are produced in the pilot plant, and the data obtained are shown in the following table.

Strength	Percent Hardwood	Strength	Percent Hardwood
160	10	181	20
171	15	188	25
175	15	193	25
182	20	195	28
184	20	200	30

(a) Fit a linear regression model relating strength to percent hardwood.
(b) Test the model in part (a) for significance of regression.
(c) Find a 95 percent confidence interval on the parameter β_1.

10-2. A plant distills liquid air to produce oxygen, nitrogen, and argon. The percentage of impurity in the oxygen is thought to be linearly related to the amount of impurities in

the air as measured by the "pollution count" in parts per million (ppm). A sample of plant operating data is shown below:

Purity (%)	93.3	92.0	92.4	91.7	94.0	94.6	93.6
Pollution count (ppm)	1.10	1.45	1.36	1.59	1.08	0.75	1.20
93.1	93.2	92.9	92.2	91.3	90.1	91.6	91.9
0.99	0.83	1.22	1.47	1.81	2.03	1.75	1.68

(a) Fit a linear regression model to the data.
(b) Test for significance of regression.
(c) Find a 95 percent confidence interval on β_1.

10-3. Plot the residuals from Problem 10-1 and comment on model adequacy.

10-4. Plot the residuals from Problem 10-2 and comment on model adequacy.

10-5. Using the results of Problem 10-1, test the regression model for lack of fit.

10-6. A study was performed on wear of a bearing y and its relationship to x_1 = oil viscosity and x_2 = load. The following data were obtained:

y	x_1	x_2
193	1.6	851
230	15.5	816
172	22.0	1058
91	43.0	1201
113	33.0	1357
125	40.0	1115

(a) Fit a multiple linear regression model to the data.
(b) Test for significance of regression.
(c) Compute t statistics for each model parameter. What conclusions can you draw?

10-7. The brake horsepower developed by an automobile engine on a dynomometer is thought to be a function of the engine speed in revolutions per minute (rpm), the road octane number of the fuel, and the engine compression. An experiment is run in the laboratory and the data that follow are collected:

Brake Horsepower	rpm	Road Octane Number	Compression
225	2000	90	100
212	1800	94	95
229	2400	88	110
222	1900	91	96
219	1600	86	100
278	2500	96	110
246	3000	94	98
237	3200	90	100
233	2800	88	105
224	3400	86	97
223	1800	90	100
230	2500	89	104

(a) Fit a multiple regression model to these data.
(b) Test for significance of regression. What conclusions can you draw?
(c) Based on t tests, do you need all three regressor variables in the model?

10-8. Analyze the residuals from the regression model in Problem 10-7. Comment on model adequacy.

10-9. The yield of a chemical process is related to the concentration of the reactant and the operating temperature. An experiment has been conducted with the following results.

Yield	Concentration	Temperature
81	1.00	150
89	1.00	180
83	2.00	150
91	2.00	180
79	1.00	150
87	1.00	180
84	2.00	150
90	2.00	180

(a) Suppose we wish to fit a main effects model to this data. Set up the $\mathbf{X}'\mathbf{X}$ matrix using the data exactly as it appears in the table.
(b) Is the matrix you obtained in part (a) diagonal? Discuss your response.
(c) Suppose we write our model in terms of the "usual" coded variables

$$x_1 = \frac{\text{Conc} - 1.5}{0.5} \qquad x_2 = \frac{\text{Temp} - 165}{15}$$

Set up the $\mathbf{X}'\mathbf{X}$ matrix for the model in terms of these coded variables. Is this matrix diagonal? Discuss your response.
(d) Define a new set of coded variables

$$x_1 = \frac{\text{Conc} - 1.0}{1.0} \qquad x_2 = \frac{\text{Temp} - 150}{30}$$

Set up the $\mathbf{X}'\mathbf{X}$ matrix for the model in terms of this set of coded variables. Is this matrix diagonal? Discuss your response.
(e) Summarize what you have learned from this problem about coding the variables.

10-10. Consider the 2^4 factorial experiment in Example 6-2. Suppose that the last observation is missing. Reanalyze the data and draw conclusions. How do these conclusions compare with those from the original example?

10-11. Consider the 2^4 factorial experiment in Example 6-2. Suppose that the last two observations are missing. Reanalyze the data and draw conclusions. How do these conclusions compare with those from the original example?

10-12. Given the following data, fit the second-order polynomial regression model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \epsilon$$

y	x_1	x_2
26	1.0	1.0
24	1.0	1.0
175	1.5	4.0
160	1.5	4.0
163	1.5	4.0
55	0.5	2.0
62	1.5	2.0
100	0.5	3.0
26	1.0	1.5
30	0.5	1.5
70	1.0	2.5
71	0.5	2.5

After you have fit the model, test for significance of regression.

10-13. (a) Consider the quadratic regression model from Problem 10-12. Compute t statistics for each model parameter and comment on the conclusions that follow from these quantities.

(b) Use the extra sum of squares method to evaluate the value of the quadratic terms x_1^2, x_2^2, and x_1x_2 to the model.

10-14. ***Relationship between analysis of variance and regression.*** Any analysis of variance model can be expressed in terms of the general linear model $\mathbf{y} = \mathbf{x}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, where the $\mathbf{X}$ matrix consists of 0s and 1s. Show that the single-factor model $y_{ij} = \mu + \tau_i + \epsilon_{ij}$, $i = 1, 2, 3, j = 1, 2, 3, 4$ can be written in general linear model form. Then

(a) Write the normal equations $(\mathbf{X}'\mathbf{X})\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{y}$ and compare them with the normal equations found for this model in Chapter 3.

(b) Find the rank of $\mathbf{X}'\mathbf{X}$. Can $(\mathbf{X}'\mathbf{X})^{-1}$ be obtained?

(c) Suppose the first normal equation is deleted and the restriction $\sum_{i=1}^{3} n\hat{\tau}_i = 0$ is added. Can the resulting system of equations be solved? If so, find the solution. Find the regression sum of squares $\hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y}$, and compare it to the treatment sum of squares in the single-factor model.

10-15. Suppose that we are fitting a straight line and we desire to make the variance of $\hat{\beta}_1$ as small as possible. Restricting ourselves to an even number of experimental points, where should we place these points so as to minimize $V(\hat{\beta}_1)$? [Note: Use the design called for in this exercise with *great* caution because, even though it minimizes $V(\hat{\beta}_1)$, it has some undesirable properties; for example, see Myers and Montgomery (1995). Only if you are *very sure* the true functional relationship is linear should you consider using this design.]

10-16. ***Weighted least squares.*** Suppose that we are fitting the straight line $y = \beta_0 + \beta_1 x + \epsilon$, but the variance of the y's now depends on the level of x; that is,

$$V(y|x_i) = \sigma_i^2 = \frac{\sigma^2}{w_i} \qquad i = 1, 2, \ldots, n$$

where the w_i are known constants, often called weights. Show that if we choose estimates of the regression coefficients to minimize the weighted sum of squared errors given by $\sum_{i=1}^{n} w_i(y_i - \beta_0 - \beta_1 x_i)^2$, the resulting least squares normal equations are

$$\hat{\beta}_0 \sum_{i=1}^{n} w_i + \hat{\beta}_1 \sum_{i=1}^{n} w_i x_i = \sum_{i=1}^{n} w_i y_i$$

$$\hat{\beta}_0 \sum_{i=1}^{n} w_i x_i + \hat{\beta}_1 \sum_{i=1}^{n} w_i x_i^2 = \sum_{i=1}^{n} w_i x_i y_i$$

10-17. Consider the 2_{IV}^{4-1} design discussed in Example 10-5.

(a) Suppose you elect to augment the design with the single run selected in that example. Find the variances and covariances of the regression coefficients in the model (ignoring blocks):

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_{12} x_1 x_2 + \beta_{34} x_3 x_4 + \epsilon$$

(b) Are there any other runs in the alternate fraction that would de-alias AB from CD?

(c) Suppose you augment the design with the four runs suggested in Example 10-5. Find the variances and covariances of the regression coefficients (ignoring blocks) for the model in part (a).

(d) Considering parts (a) and (c), which augmentation strategy would you prefer, and why?

10-18. Consider a 2_{III}^{7-4} design. Suppose after running the experiment, the largest observed effects are $A + BD$, $B + AD$, and $D + AB$. You wish to augment the original design with a group of four runs to de-alias these effects.

(a) Which four runs would you make?

(b) Find the variances and covariances of the regression coefficients in the model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_4 x_4 + \beta_{12} x_1 x_2 + \beta_{14} x_1 x_4 + \beta_{24} x_2 x_4 + \epsilon.$$

(c) Is it possible to de-alias these effects with fewer than four additional runs?

11 Response Surface Methods and Other Approaches to Process Optimization

11-1 INTRODUCTION TO RESPONSE SURFACE METHODOLOGY

Response surface methodology, or **RSM**, is a collection of mathematical and statistical techniques that are useful for the modeling and analysis of problems in which a response of interest is influenced by several variables and the objective is to optimize this response. For example, suppose that a chemical engineer wishes to find the levels of temperature (x_1) and pressure (x_2) that maximize the yield (y) of a process. The process yield is a function of the levels of temperature and pressure, say

$$y = f(x_1, x_2) + \epsilon$$

where ϵ represents the noise or error observed in the response y. If we denote the expected response by $E(y) = f(x_1, x_2) = \eta$, then the surface represented by

$$\eta = f(x_1, x_2)$$

is called a **response surface**.

We usually represent the response surface graphically, such as in Figure 11-1 (on the next page), where η is plotted versus the levels of x_1 and x_2. We have seen response surface plots such as this before, particularly in the chapters on factorial designs. To help visualize the shape of a response surface, we often plot the contours of the response surface as shown in Figure 11-2 (on the next page). In the contour plot, lines of constant response are drawn in the x_1, x_2 plane. Each contour corresponds to a particular height of the response surface. We have also previously seen the utility of contour plots.

In most RSM problems, the form of the relationship between the response and the independent variables is unknown. Thus, the first step in RSM is to find a suitable approximation for the true functional relationship between y and the set of independent variables. Usually, a low-order polynomial in some region of the independent variables is employed. If the response is well modeled by a linear function of the independent variables, then the approximating function is the **first-order model**

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \epsilon \qquad (11\text{-}1)$$

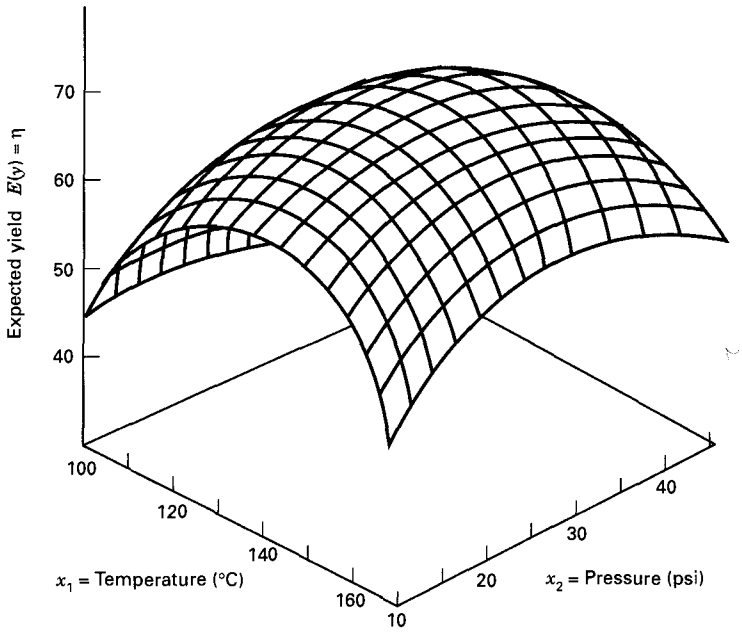


Figure 11-1 A three-dimensional response surface showing the expected yield (η) as a function of temperature (x_1) and pressure (x_2).

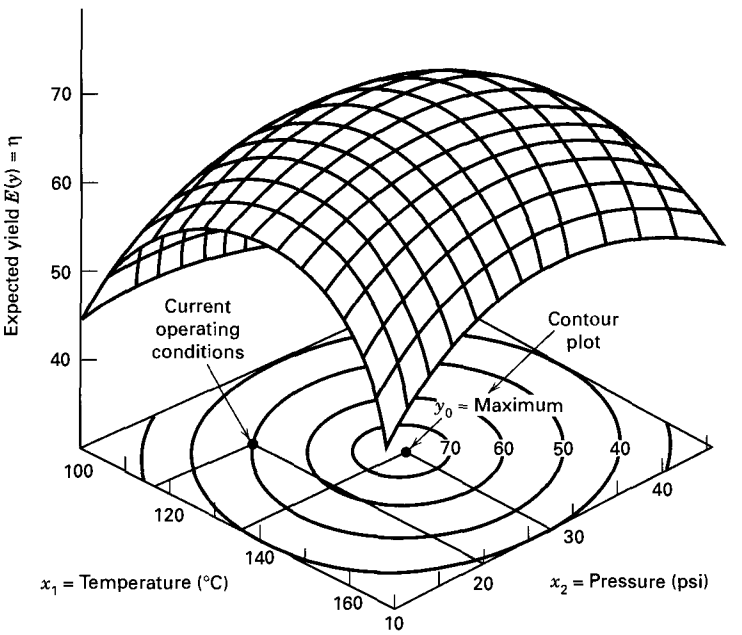


Figure 11-2 A contour plot of a response surface.

If there is curvature in the system, then a polynomial of higher degree must be used, such as the **second-order model**

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum\sum_{i<j} \beta_{ij} x_i x_j + \epsilon \tag{11-2}$$

Almost all RSM problems use one or both of these models. Of course, it is unlikely that a polynomial model will be a reasonable approximation of the true functional relationship over the entire space of the independent variables, but for a relatively small region they usually work quite well.

The method of least squares, discussed in Chapter 10, is used to estimate the parameters in the approximating polynomials. The response surface analysis is then performed using the fitted surface. If the fitted surface is an adequate approximation of the true response function, then analysis of the fitted surface will be approximately equivalent to analysis of the actual system. The model parameters can be estimated most effectively if proper experimental designs are used to collect the data. Designs for fitting response surfaces are called **response surface designs**. These designs are discussed in Section 11-4.

RSM is a **sequential procedure**. Often, when we are at a point on the response surface that is remote from the optimum, such as the current operating conditions in Figure 11-3, there is little curvature in the system and the first-order model will be appropriate. Our objective here is to lead the experimenter rapidly and efficiently along a path of improvement toward the general vicinity of the **optimum**. Once the region of the optimum has been found, a more elaborate model, such as the second-order model, may be employed, and an analysis may be performed to locate the optimum. From Figure 11-3, we see that the analysis of a response surface can be thought of as "climbing a hill," where the top of the hill represents the point of maximum response. If the true optimum is a point of minimum response, then we may think of "descending into a valley."

The eventual objective of RSM is to determine the optimum operating conditions for the system or to determine a region of the factor space in which operating require-

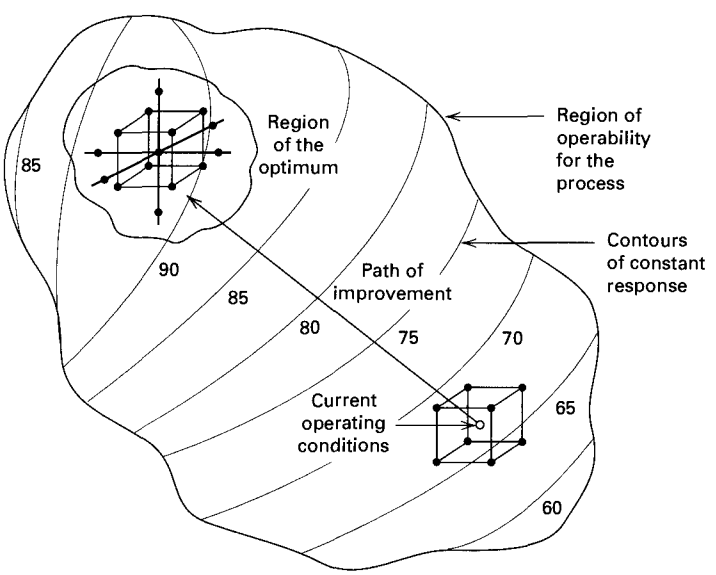


Figure 11-3 The sequential nature of RSM.

ments are satisfied. More extensive presentations of RSM are in Myers and Montgomery (1995), Khuri and Cornell (1996), and Box and Draper (1987).

11-2 THE METHOD OF STEEPEST ASCENT

Frequently, the initial estimate of the optimum operating conditions for the system will be far from the actual optimum. In such circumstances, the objective of the experimenter is to move rapidly to the general vicinity of the optimum. We wish to use a simple and economically efficient experimental procedure. When we are remote from the optimum, we usually assume that a first-order model is an adequate approximation to the true surface in a small region of the x's.

The **method of steepest ascent** is a procedure for moving sequentially along the path of steepest ascent, that is, in the direction of the maximum increase in the response. Of course, if minimization is desired, then we call this technique the **method of steepest descent**. The fitted first-order model is

$$\hat{y} = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i \tag{11-3}$$

and the first-order response surface, that is, the contours of $\hat{y}$, is a series of parallel lines such as that shown in Figure 11-4. The direction of steepest ascent is the direction in which $\hat{y}$ increases most rapidly. This direction is parallel to the normal to the fitted response surface. We usually take as the **path of steepest ascent** the line through the center of the region of interest and normal to the fitted surface. Thus, the steps along the

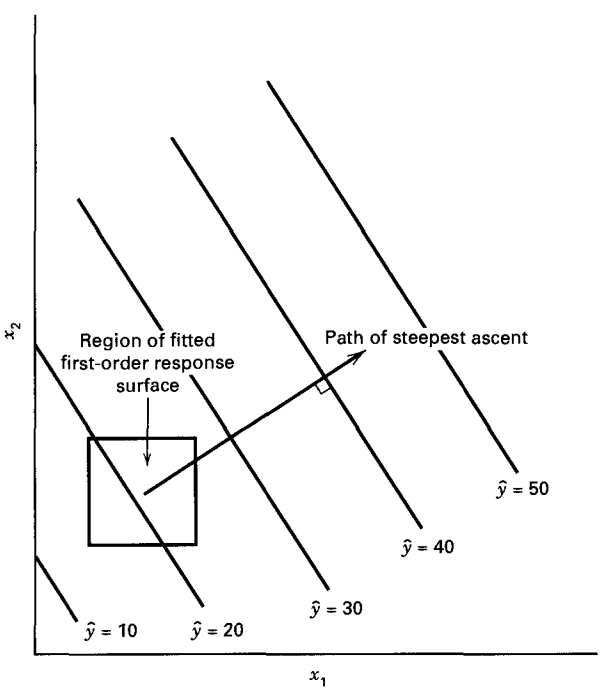


Figure 11-4 First-order response surface and path of steepest ascent.

path are proportional to the regression coefficients $\{\hat{\beta}_i\}$. The actual step size is determined by the experimenter based on process knowledge or other practical considerations.

Experiments are conducted along the path of steepest ascent until no further increase in response is observed. Then a new first-order model may be fit, a new path of steepest ascent determined, and the procedure continued. Eventually, the experimenter will arrive in the vicinity of the optimum. This is usually indicated by lack of fit of a first-order model. At that time additional experiments are conducted to obtain a more precise estimate of the optimum.

EXAMPLE 11-1

A chemical engineer is interested in determining the operating conditions that maximize the yield of a process. Two controllable variables influence process yield: reaction time and reaction temperature. The engineer is currently operating the process with a reaction time of 35 minutes and a temperature of 155°F, which result in yields of around 40 percent. Because it is unlikely that this region contains the optimum, she fits a first-order model and applies the method of steepest ascent.

The engineer decides that the region of exploration for fitting the first-order model should be (30, 40) minutes of reaction time and (150, 160)°F. To simplify the calculations, the independent variables will be coded to the usual (−1, 1) interval. Thus, if ξ_1 denotes the **natural variable** time and ξ_2 denotes the **natural variable** temperature, then the **coded variables** are

$$x_1 = \frac{\xi_1 - 35}{5} \quad \text{and} \quad x_2 = \frac{\xi_2 - 155}{5}$$

The experimental design is shown in Table 11-1. Note that the design used to collect this data is a 2^2 factorial augmented by five center points. Replicates at the center are used to estimate the experimental error and to allow for checking the adequacy of the first-order model. Also, the design is centered about the current operating conditions for the process.

A first-order model may be fit to these data by least squares. Following the methods for two-level designs, we obtain the following model in the coded variables:

$$\hat{y} = 40.44 + 0.775x_1 + 0.325x_2$$

Table 11-1 Process Data for Fitting the First-Order Model

Natural Variables		Coded Variables		Response
ξ_1	ξ_2	x_1	x_2	y
30	150	−1	−1	39.3
30	160	−1	1	40.0
40	150	1	−1	40.9
40	160	1	1	41.5
35	155	0	0	40.3
35	155	0	0	40.5
35	155	0	0	40.7
35	155	0	0	40.2
35	155	0	0	40.6

Before exploring along the path of steepest ascent, the adequacy of the first-order model should be investigated. The 2^2 design with center points allows the experimenter to

1. Obtain an estimate of error
2. Check for interactions (cross-product terms) in the model
3. Check for quadratic effects (curvature)

The replicates at the center can be used to calculate an estimate of error as follows:

$$\hat{\sigma}^2 = \frac{(40.3)^2 + (40.5)^2 + (40.7)^2 + (40.2)^2 + (40.6)^2 - (202.3)^2/5}{4}$$
$$= 0.0430$$

The first-order model assumes that the variables x_1 and x_2 have an **additive effect** on the response. Interaction between the variables would be represented by the coefficient β_{12} of a cross-product term x_1x_2 added to the model. The least squares estimate of this coefficient is just one-half the interaction effect calculated as in an ordinary 2^2 factorial design, or

$$\hat{\beta}_{12} = \tfrac{1}{4}[(1 \times 39.3) + (1 \times 41.5) + (-1 \times 40.0) + (-1 \times 40.9)]$$
$$= \tfrac{1}{4}(-0.1)$$
$$= -0.025$$

The single degree of freedom sum of squares for interaction is

$$SS_{\text{Interaction}} = \frac{(-0.1)^2}{4}$$
$$= 0.0025$$

Comparing $SS_{\text{Interaction}}$ to $\hat{\sigma}^2$ gives a lack-of-fit statistic

$$F = \frac{SS_{\text{Interaction}}}{\hat{\sigma}^2}$$
$$= \frac{0.0025}{0.0430}$$
$$= 0.058$$

which is small, indicating that interaction is negligible.

Another check of the adequacy of the straight-line model is obtained by applying the check for pure quadratic curvature effect described in Section 6-6. Recall that this consists of comparing the average response at the four points in the factorial portion of the design, say $\bar{y}_F = 40.425$, with the average response at the design center, say $\bar{y}_C = 40.46$. If there is quadratic curvature in the true response function, then $\bar{y}_F - \bar{y}_C$ is a measure of this curvature. If β_{11} and β_{22} are the coefficients of the "pure quadratic" terms x_1^2 and x_2^2, then $\bar{y}_F - \bar{y}_C$ is an estimate of $\beta_{11} + \beta_{22}$. In our example, an estimate of the pure quadratic term is

$$\hat{\beta}_{11} + \hat{\beta}_{22} = \bar{y}_F - \bar{y}_C$$
$$= 40.425 - 40.46$$
$$= -0.035$$

Table 11-2 Analysis of Variance for the First-Order Model

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Model (β_1, β_2)	2.8250	2	1.4125	47.83	0.0002
Residual	0.1772	6			
(Interaction)	(0.0025)	1	0.0025	0.058	0.8215
(Pure quadratic)	(0.0027)	1	0.0027	0.063	0.8142
(Pure error)	(0.1720)	4	0.0430		
Total	3.0022	8			

The single-degree-of-freedom sum of squares associated with the null hypothesis, $H_0: \beta_{11} + \beta_{22} = 0$, is

$$\begin{aligned} SS_{\text{Pure Quadratic}} &= \frac{n_F n_C (\bar{y}_F - \bar{y}_C)^2}{n_F + n_C} \\ &= \frac{(4)(5)(-0.035)^2}{4 + 5} \\ &= 0.0027 \end{aligned}$$

where n_F and n_C are the number of points in the factorial portion and the number of center points, respectively. Because

$$\begin{aligned} F &= \frac{SS_{\text{Pure Quadratic}}}{\hat{\sigma}^2} \\ &= \frac{0.0027}{0.0430} \\ &= 0.063 \end{aligned}$$

is small, there is no indication of a pure quadratic effect.

The analysis of variance for this model is summarized in Table 11-2. Both the interaction and curvature checks are not significant, whereas the F test for the overall regression is significant. Furthermore, the standard error of $\hat{\beta}_1$ and $\hat{\beta}_2$ is

$$se(\hat{\beta}_i) = \sqrt{\frac{MS_E}{4}} = \sqrt{\frac{\hat{\sigma}^2}{4}} = \sqrt{\frac{0.0430}{4}} = 0.10 \qquad i = 1, 2$$

Both regression coefficients $\hat{\beta}_1$ and $\hat{\beta}_2$ are large relative to their standard errors. At this point, we have no reason to question the adequacy of the first-order model.

To move away from the design center—the point ($x_1 = 0$, $x_2 = 0$)—along the path of steepest ascent, we would move 0.775 units in the x_1 direction for every 0.325 units in the x_2 direction. Thus, the path of steepest ascent passes through the point ($x_1 = 0$, $x_2 = 0$) and has a slope 0.325/0.775. The engineer decides to use 5 minutes of reaction time as the basic step size. Using the relationship between ξ_1 and x_1, we see that 5 minutes of reaction time is equivalent to a step in the *coded* variable x_1 of $\Delta x_1 = 1$. Therefore, the steps along the path of steepest ascent are $\Delta x_1 = 1.0000$ and $\Delta x_2 = (0.325/0.775)\,\Delta x_1 = 0.42$.

The engineer computes points along this path and observes the yields at these points until a decrease in response is noted. The results are shown in Table 11-3 (on the next page) in both coded and natural variables. Although the coded variables are easier to manipulate mathematically, the natural variables must be used in running the process.

Table 11-3 Steepest Ascent Experiment for Example 11-1

Steps	Coded Variables		Natural Variables		Response
	x_1	x_2	ξ_1	ξ_2	y
Origin	0	0	35	155	
Δ	1.00	0.42	5	2	
Origin + Δ	1.00	0.42	40	157	41.0
Origin + 2Δ	2.00	0.84	45	159	42.9
Origin + 3Δ	3.00	1.26	50	161	47.1
Origin + 4Δ	4.00	1.68	55	163	49.7
Origin + 5Δ	5.00	2.10	60	165	53.8
Origin + 6Δ	6.00	2.52	65	167	59.9
Origin + 7Δ	7.00	2.94	70	169	65.0
Origin + 8Δ	8.00	3.36	75	171	70.4
Origin + 9Δ	9.00	3.78	80	173	77.6
Origin + 10Δ	10.00	4.20	85	175	80.3
Origin + 11Δ	11.00	4.62	90	179	76.2
Origin + 12Δ	12.00	5.04	95	181	75.1

Figure 11-5 plots the yield at each step along the path of steepest ascent. Increases in response are observed through the tenth step; however, all steps beyond this point result in a decrease in yield. Therefore, another first-order model should be fit in the general vicinity of the point ($\xi_1 = 85$, $\xi_2 = 175$).

A new first-order model is fit around the point ($\xi_1 = 85$, $\xi_2 = 175$). The region of exploration for ξ_1 is [80, 90], and for ξ_2 it is [170, 180]. Thus, the coded variables are

$$x_1 = \frac{\xi_1 - 85}{5} \quad \text{and} \quad x_2 = \frac{\xi_2 - 175}{5}$$

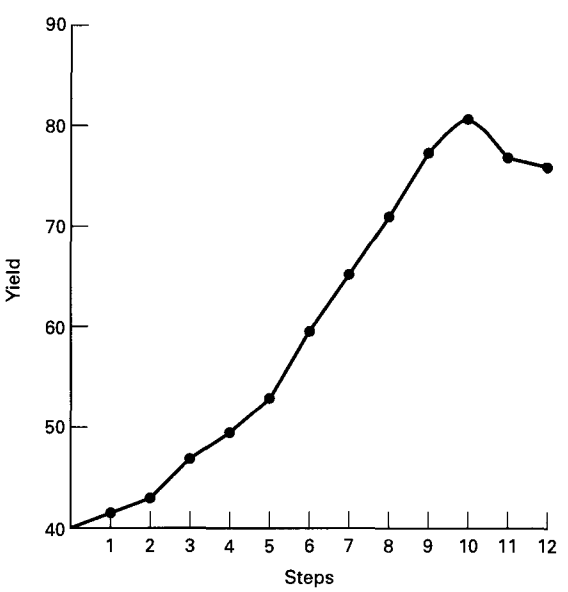


Figure 11-5 Yield versus steps along the path of steepest ascent for Example 11-1.

Table 11-4 Data for Second First-Order Model

Natural Variables		Coded Variables		Response
ξ_1	ξ_2	x_1	x_2	y
80	170	−1	−1	76.5
80	180	−1	1	77.0
90	170	1	−1	78.0
90	180	1	1	79.5
85	175	0	0	79.9
85	175	0	0	80.3
85	175	0	0	80.0
85	175	0	0	79.7
85	175	0	0	79.8

Once again, a 2^2 design with five center points is used. The experimental design is shown in Table 11-4.

The first-order model fit to the coded variables in Table 11-4 is

$$\hat{y} = 78.97 + 1.00x_1 + 0.50x_2$$

The analysis of variance for this model, including the interaction and pure quadratic term checks, is shown in Table 11-5. The interaction and pure quadratic checks imply that the first-order model is not an adequate approximation. This curvature in the true surface may indicate that we are near the optimum. At this point, additional analysis must be done to locate the optimum more precisely.

From Example 11-1 we notice that the *path of steepest ascent is proportional to the signs and magnitudes of the regression coefficients* in the fitted first-order model

$$\hat{y} = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i$$

It is easy to give a general algorithm for determining the coordinates of a point on the path of steepest ascent. Assume that the point $x_1 = x_2 = \ldots = x_k = 0$ is the base or origin point. Then

1. Choose a step size in one of the process variables, say Δx_j. Usually, we would select the variable we know the most about, or we would select the variable that has the largest absolute regression coefficient $|\hat{\beta}_j|$.

Table 11-5 Analysis of Variance for the Second First-Order Model

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Regression	5.00	2			
Residual	11.1200	6			
(Interaction)	(0.2500)	1	0.2500	4.72	0.0955
(Pure quadratic)	(10.6580)	1	10.6580	201.09	0.0001
(Pure error)	(0.2120)	4	0.0530		
Total	16.1200	8			

2. The step size in the other variables is

$$\Delta x_i = \frac{\hat{\beta}_i}{\hat{\beta}_j/\Delta x_j} \qquad i = 1, 2, \ldots, k; \qquad i \neq j$$

3. Convert the Δx_i from coded variables to the natural variables.

To illustrate, consider the path of steepest ascent computed in Example 11-1. Because x_1 has the largest regression coefficient, we select reaction time as the variable in step 1 of the above procedure. Five minutes of reaction time is the step size (based on process knowledge). In terms of the coded variables, this is $\Delta x_1 = 1.0$. Therefore, from guideline 2, the step size in temperature is

$$\Delta x_2 = \frac{\hat{\beta}_2}{\hat{\beta}_1/\Delta x_1} = \frac{0.325}{(0.775/1.0)} = 0.42$$

To convert the coded step sizes ($\Delta x_1 = 1.0$ and $\Delta x_2 = 0.42$) to the natural units of time and temperature, we use the relationships

$$\Delta x_1 = \frac{\Delta \xi_1}{5} \qquad \text{and} \qquad \Delta x_2 = \frac{\Delta \xi_2}{5}$$

which results in

$$\Delta \xi_1 = \Delta x_1(5) = 1.0(5) = 5 \text{ min}$$

and

$$\Delta \xi_2 = \Delta x_2(5) = 0.42(5) = 2°\text{F}$$

11-3 ANALYSIS OF A SECOND-ORDER RESPONSE SURFACE

When the experimenter is relatively close to the optimum, a model that incorporates curvature is usually required to approximate the response. In most cases, the second-order model

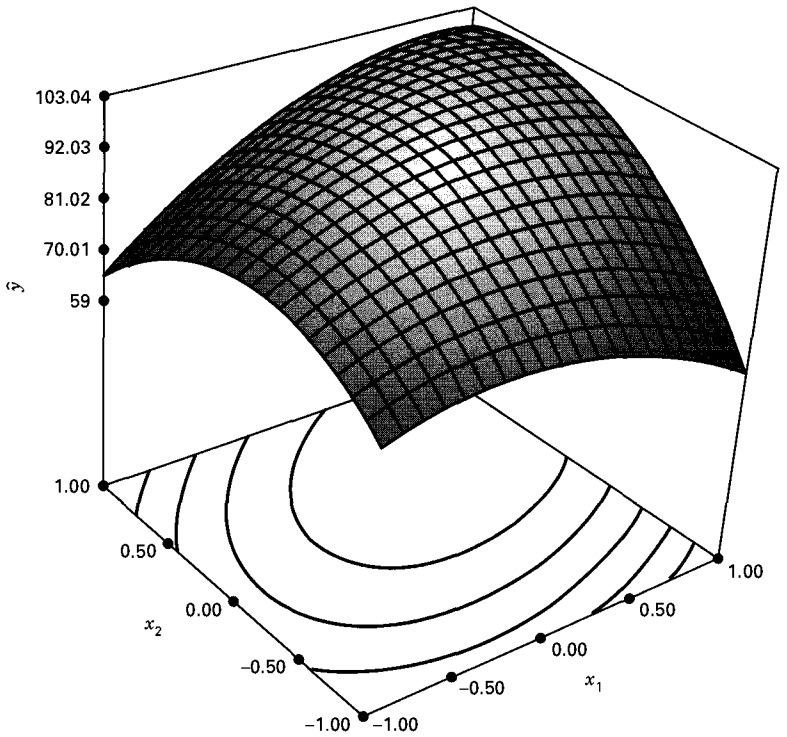
$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum\sum_{i<j} \beta_{ij} x_i x_j + \epsilon \tag{11-4}$$

is adequate. In this section we will show how to use this fitted model to find the optimum set of operating conditions for the x's and to characterize the nature of the response surface.

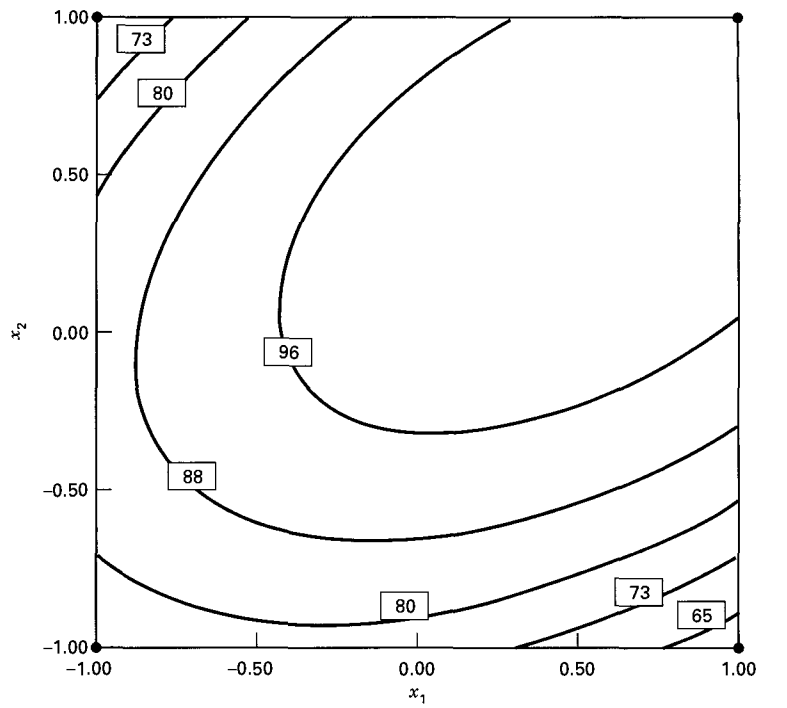
11-3.1 Location of the Stationary Point

Suppose we wish to find the levels of $x_1, x_2, \ldots, x_k$ that optimize the predicted response. This point, if it exists, will be the set of $x_1, x_2, \ldots, x_k$ for which the partial derivatives $\partial \hat{y}/\partial x_1 = \partial \hat{y}/\partial x_2 = \cdots = \partial \hat{y}/\partial x_k = 0$. This point, say $x_{1,s}, x_{2,s}, \ldots, x_{k,s}$, is called the **stationary point**. The stationary point could represent (1) a point of **maximum response**, (2) a point of **minimum response**, or (3) a **saddle point**. These three possibilities are shown in Figures 11-6, 11-7 (page 438), and 11-8 (page 439).

Contour plots play a very important role in the study of the response surface. By generating contour plots using computer software for response surface analysis, the ex-

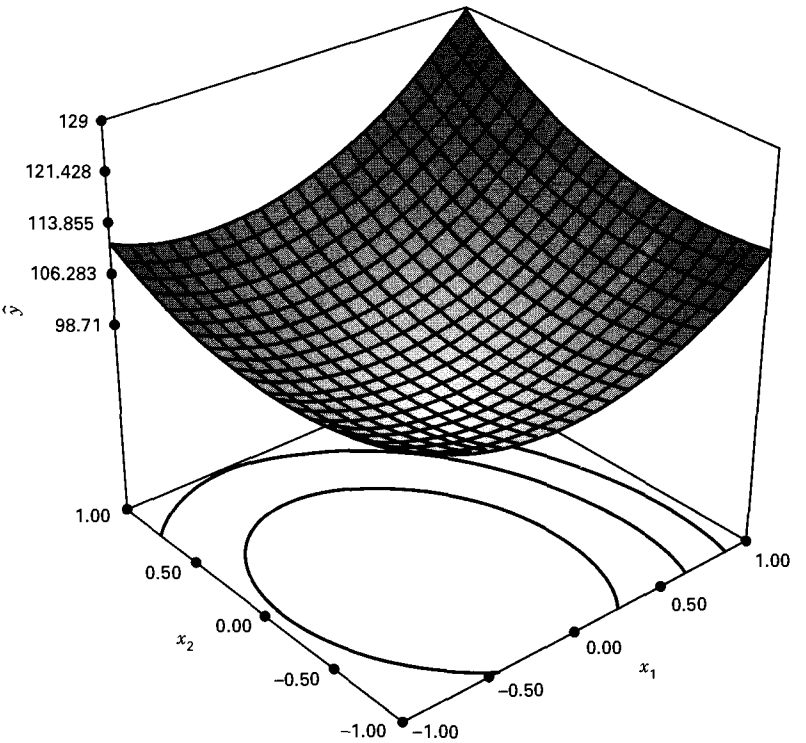


(*a*) Response surface

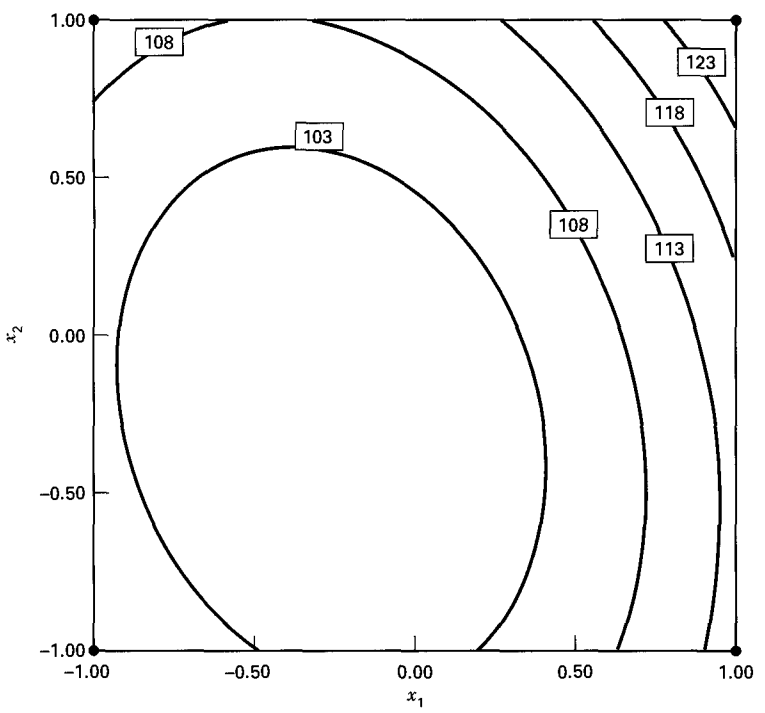


(*b*) Contour plot

Figure 11-6 Response surface and contour plot illustrating a surface with a maximum.

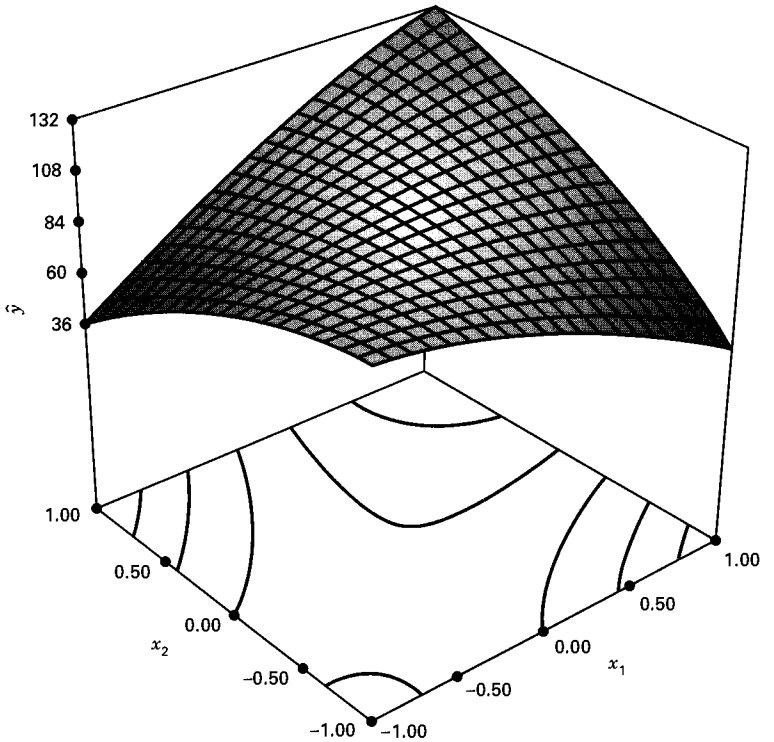


(*a*) Response surface

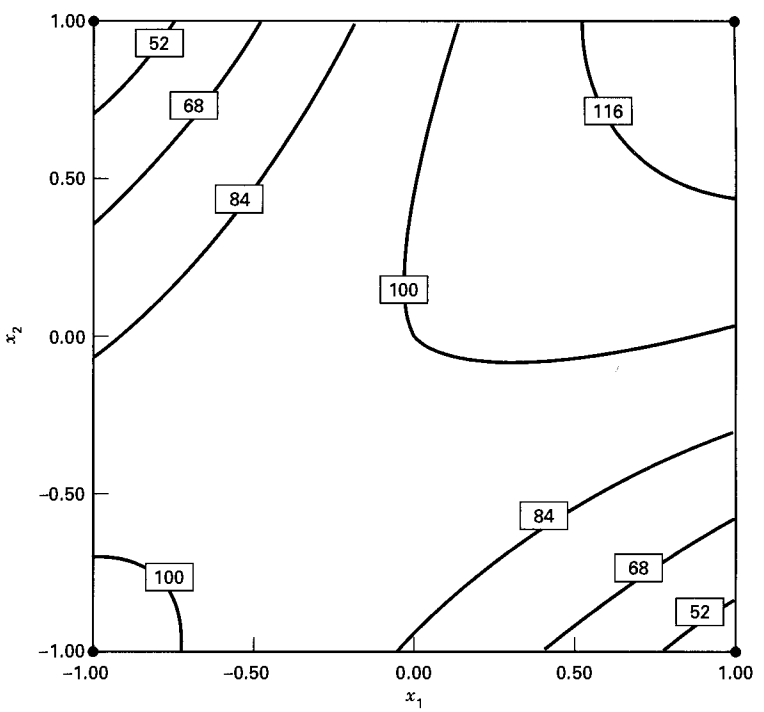


(*b*) Contour plot

Figure 11-7 Response surface and contour plot illustrating a surface with a minimum.



(*a*) Response surface



(*b*) Contour plot

Figure 11-8 Response surface and contour plot illustrating a saddle point (or minimax).

perimenter can usually characterize the shape of the surface and locate the optimum with reasonable precision.

We may obtain a general mathematical solution for the location of the stationary point. Writing the second-order model in matrix notation, we have

$$\hat{y} = \hat{\beta}_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x} \tag{11-5}$$

where

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} \qquad \text{and} \qquad \mathbf{B} = \begin{bmatrix} \hat{\beta}_{11}, \hat{\beta}_{12}/2, \ldots, \hat{\beta}_{1k}/2 \\ \hat{\beta}_{22}, \ldots, \hat{\beta}_{2k}/2 \\ \ddots \\ \text{sym.} \qquad \hat{\beta}_{kk} \end{bmatrix}$$

That is, $\mathbf{b}$ is a $(k \times 1)$ vector of the first-order regression coefficients and $\mathbf{B}$ is a $(k \times k)$ symmetric matrix whose main diagonal elements are the *pure* quadratic coefficients $(\hat{\beta}_{ii})$ and whose off-diagonal elements are one-half the *mixed* quadratic coefficients $(\hat{\beta}_{ij}, i \neq j)$. The derivative of $\hat{y}$ with respect to the elements of the vector $\mathbf{x}$ equated to $\mathbf{0}$ is

$$\frac{\partial \hat{y}}{\partial \mathbf{x}} = \mathbf{b} + 2\mathbf{B}\mathbf{x} = \mathbf{0} \tag{11-6}$$

The stationary point is the solution to Equation 11-6, or

$$\mathbf{x}_s = -\tfrac{1}{2}\mathbf{B}^{-1}\mathbf{b} \tag{11-7}$$

Furthermore, by substituting Equation 11-7 into Equation 11-5, we can find the predicted response at the stationary point as

$$\hat{y}_s = \hat{\beta}_0 + \tfrac{1}{2}\mathbf{x}_s'\mathbf{b} \tag{11-8}$$

11-3.2 Characterizing the Response Surface

Once we have found the stationary point, it is usually necessary to characterize the response surface in the immediate vicinity of this point. By **characterize**, we mean determine whether the stationary point is a point of maximum or minimum response or a saddle point. We also usually want to study the relative sensitivity of the response to the variables $x_1, x_2, \ldots, x_k$.

As we mentioned previously, the most straightforward way to do this is to examine a **contour plot** of the fitted model. If there are only two or three process variables (the x's), the construction and interpretation of this contour plot is relatively easy. However, even when there are relatively few variables, a more formal analysis, called the **canonical analysis**, can be useful.

It is helpful first to transform the model into a new coordinate system with the origin at the stationary point $\mathbf{x}_s$ and then to rotate the axes of this system until they are parallel to the principal axes of the fitted response surface. This transformation is illustrated in Figure 11-9 on the facing page. We can show that this results in the fitted model

$$\hat{y} = \hat{y}_s + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \cdots + \lambda_k w_k^2 \tag{11-9}$$

where the $\{w_i\}$ are the transformed independent variables and the $\{\lambda_i\}$ are constants. Equation 11-9 is called the **canonical form** of the model. Furthermore, the $\{\lambda_i\}$ are just the **eigenvalues** or **characteristic roots** of the matrix $\mathbf{B}$.

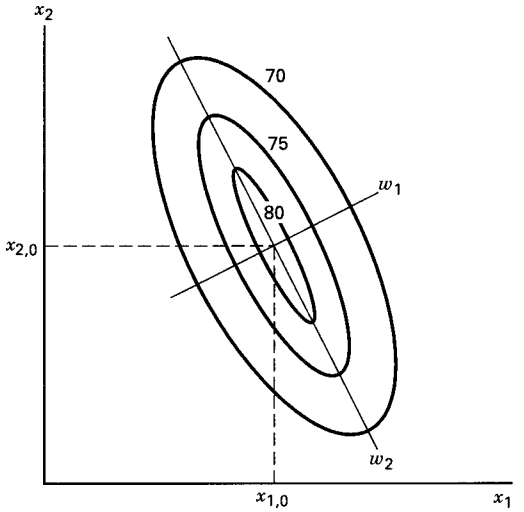


Figure 11-9 Canonical form of the second-order model.

The nature of the response surface can be determined from the stationary point and the *signs* and *magnitudes* of the $\{\lambda_i\}$. First, suppose that the stationary point is within the region of exploration for fitting the second-order model. If the $\{\lambda_i\}$ are all positive, $\mathbf{x}_s$ is a point of minimum response; if the $\{\lambda_i\}$ are all negative, $\mathbf{x}_s$ is a point of maximum response; and if the $\{\lambda_i\}$ have different signs, $\mathbf{x}_s$ is a saddle point. Furthermore, the surface is steepest in the w_i direction for which $|\lambda_i|$ is the greatest. For example, Figure 11-9 depicts a system for which $\mathbf{x}_s$ is a maximum (λ_1 and λ_2 are negative) with $|\lambda_1| > |\lambda_2|$.

EXAMPLE 11-2

We will continue the analysis of the chemical process in Example 11-1. A second-order model in the variables x_1 and x_2 cannot be fit using the design in Table 11-4. The experimenter decides to augment this design with enough points to fit a second-order model.[1] She obtains four observations at ($x_1 = 0$, $x_2 = \pm 1.414$) and ($x_1 = \pm 1.414$, $x_2 = 0$). The complete experiment is shown in Table 11-6 (page 442), and the design is displayed in Figure 11-10 (on the next page). This design is called a **central composite design** (or a CCD) and will be discussed in more detail in Section 11-4.2. In this second phase of the study, two additional responses were of interest, the viscosity and the molecular weight of the product. The responses are also shown in Table 11-6.

We will focus on fitting a quadratic model to the yield response y_1 (the other responses will be discussed in Section 11-3.4). We generally use computer software to fit a response surface and to construct the contour plots. Table 11-7 (pages 443-444) contains the output from Design-Expert. From examining this table we notice that this software package first computes the "sequential or extra sums of squares" for the linear, quadratic, and cubic terms in the model (there is a warning message concerning aliasing in the cubic model because the CCD does not contain enough runs to support a full cubic

[1] The engineer ran the additional four observations at about the same time she ran the original nine observations. If substantial time had elapsed between the two sets of runs, blocking would have been necessary. Blocking in response surface designs is discussed in Section 11-4.3.

Table 11-6 Central Composite Design for Example 11-2

Natural Variables		Coded Variables		Responses		
ξ_1	ξ_2	x_1	x_2	y_1 (yield)	y_2 (viscosity)	y_3 (molecular weight)
80	170	−1	−1	76.5	62	2940
80	180	−1	1	77.0	60	3470
90	170	1	−1	78.0	66	3680
90	180	1	1	79.5	59	3890
85	175	0	0	79.9	72	3480
85	175	0	0	80.3	69	3200
85	175	0	0	80.0	68	3410
85	175	0	0	79.7	70	3290
85	175	0	0	79.8	71	3500
92.07	175	1.414	0	78.4	68	3360
77.93	175	−1.414	0	75.6	71	3020
85	182.07	0	1.414	78.5	58	3630
85	167.93	0	−1.414	77.0	57	3150

model). Based on the small P-value for the quadratic terms, we decided to fit the second-order model to the yield response. The computer output shows the final model in terms of both the coded variables and the natural or actual factor levels.

Figure 11-11 (page 445) shows the three-dimensional response surface plot and the contour plot for the yield response in terms of the process variables time and temperature. It is relatively easy to see from examining these figures that the optimum is very near 175°F and 85 minutes of reaction time and that the response is at a maximum at this point. From examination of the contour plot, we note that the process may be slightly more sensitive to changes in reaction time than to changes in temperature.

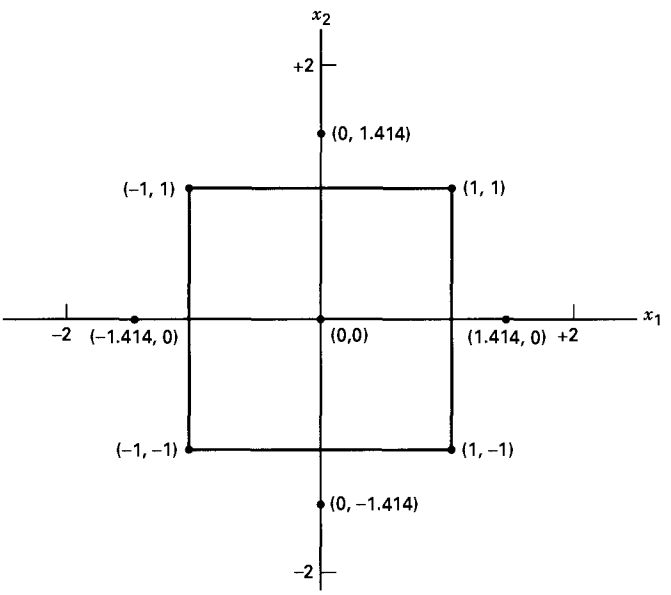


Figure 11-10 Central composite design for Example 11-2.

Table 11-7 Computer Output from Design-Expert for Fitting a Model to the Yield Response in Example 11-2

Response: yield
*****WARNING: The Cubic Model is Aliased!*****

Sequential Model Sum of Squares

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Mean	80062.16	1	80062.16			
Linear	10.04	2	5.02	2.69	0.1166	
2FI	0.25	1	0.25	0.12	0.7350	
Quadratic	*17.95*	*2*	*8.98*	*126.88*	*<0.0001*	*Suggested*
Cubic	2.042E-003	2	1.021E-003	0.010	0.9897	Aliased
Residual	0.49	5	0.099			
Total	80090.90	13	6160.84			

"*Sequential Model Sum of Squares*": Select the highest order polynomial where the additional terms are significant.

Lack of Fit Tests

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F	
Linear	18.49	6	3.08	58.14	0.0008	
2FI	18.24	5	3.65	68.82	0.0006	
Quadratic	*0.28*	*3*	*0.094*	*1.78*	*0.2897*	*Suggested*
Cubic	0.28	1	0.28	5.31	0.0826	Aliased
Pure Error	0.21	4	0.053			

"*Lack of Fit Tests*": Want the selected model to have insignificant lack-of-fit.

Model Summary Statistics

Source	Std. Dev.	R-Squared	Adjusted R-Squared	Predicted R-Squared	PRESS	
Linear	1.37	0.3494	0.2193	−0.0435	29.99	
2FI	1.43	0.3581	0.1441	−0.2730	36.59	
Quadratic	*0.27*	*0.9828*	*0.9705*	*0.9184*	*2.35*	*Suggested*
Cubic	0.31	0.9828	0.9588	0.3622	18.33	Aliased

"*Model Summary Statistics*": Focus on the model minimizing the "PRESS", or equivalently maximizing the "PRED R-SQR".

Response: yield
ANOVA for Response Surface Quadratic Model
Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	28.25	5	5.65	79.85	<0.0001
A	*7.92*	*1*	*7.92*	*111.93*	*<0.0001*
B	*2.12*	*1*	*2.12*	*30.01*	*0.0009*
A^2	*13.18*	*1*	*13.18*	*186.22*	*<0.0001*
B^2	*6.97*	*1*	*6.97*	*98.56*	*<0.0001*
AB	*0.25*	*1*	*0.25*	*3.53*	*0.1022*
Residual	0.50	7	0.071		
Lack of Fit	*0.28*	*3*	*0.094*	*1.78*	*0.2897*
Pure Error	*0.21*	*4*	*0.053*		
Cor Total	28.74	12			

Std. Dev.	0.27	R-Squared	0.9828
Mean	78.48	Adj R-Squared	0.9705
C.V.	0.34	Pred R-Squared	0.9184
PRESS	2.35	Adeq Precision	23.018

Table 11-7 (continued)

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High	VIF
Intercept	79.94	1	0.12	79.66	80.22	
A-time	0.99	1	0.094	0.77	1.22	1.00
B-temp	0.52	1	0.094	0.29	0.74	1.00
A^2	−1.38	1	0.10	−1.61	−1.14	1.02
B^2	−1.00	1	0.10	−1.24	−0.76	1.02
AB	0.25	1	0.13	−0.064	0.56	1.00

Final Equation in Terms of Coded Factors:

$$\begin{aligned} \text{yield} = \\ +79.94 \\ +0.99 * A \\ +0.52 * B \\ -1.38 * A^2 \\ -1.00 * B^2 \\ +0.25 * A * B \end{aligned}$$

Final Equation in Terms of Actual Factors:

$$\begin{aligned} \text{yield} = \\ -1430.52285 \\ +7.80749 * \text{time} \\ +13.27053 * \text{temp} \\ -0.055050 * \text{time}^2 \\ -0.040050 * \text{temp}^2 \\ +0.010000 * \text{time} * \text{temp} \end{aligned}$$

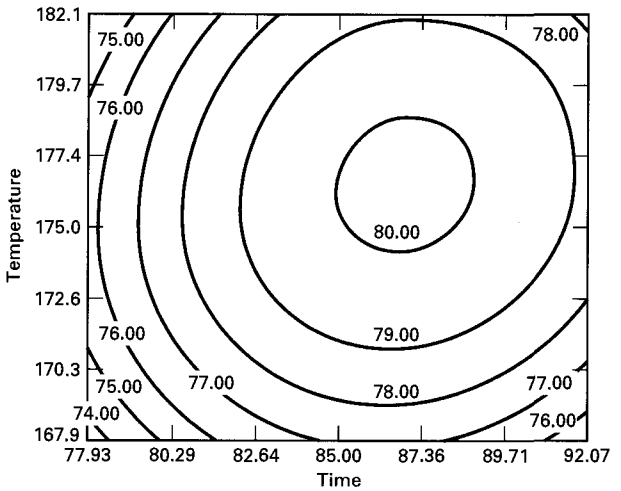
Run Order	Diagnostics Case Statistics: Standard Order	Actual Value	Predicted Value	Residual	Leverage	Student Residual	Cook's Distance	Outlier t
8	1	76.50	76.30	0.20	0.625	1.213	0.409	1.264
6	2	78.00	77.79	0.21	0.625	1.275	0.452	1.347
9	3	77.00	76.83	0.17	0.625	1.027	0.293	1.032
11	4	79.50	79.32	0.18	0.625	1.089	0.329	1.106
12	5	75.60	75.78	−0.18	0.625	−1.107	0.341	−1.129
10	6	78.40	78.59	−0.19	0.625	−1.195	0.396	−1.240
7	7	77.00	77.21	−0.21	0.625	−1.283	0.457	−1.358
1	8	78.50	78.67	−0.17	0.625	−1.019	0.289	−1.023
5	9	79.90	79.94	−0.040	0.200	−0.168	0.001	−0.156
3	10	80.30	79.94	0.36	0.200	1.513	0.095	1.708
13	11	80.00	79.94	0.060	0.200	0.252	0.003	0.235
2	12	79.70	79.94	−0.24	0.200	−1.009	0.042	−1.010
4	13	79.80	79.94	−0.14	0.200	−0.588	0.014	−0.559

We could also find the location of the stationary point using the general solution in Equation 11-7. Note that

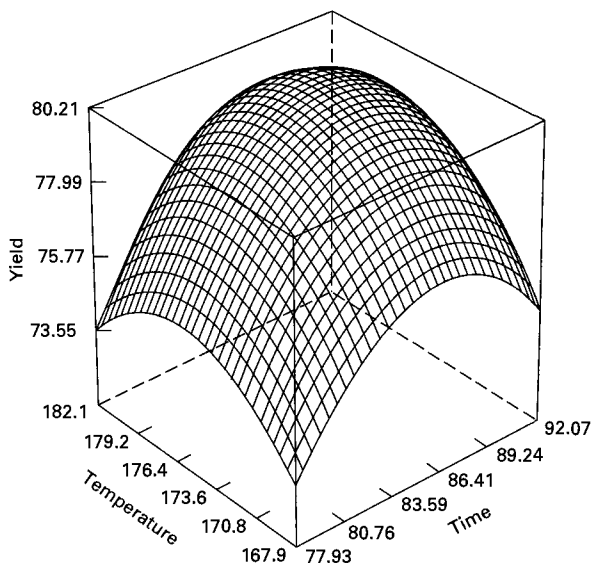
$$\mathbf{b} = \begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} -1.376 & 0.1250 \\ 0.1250 & -1.001 \end{bmatrix}$$

and from Equation 11-7 the stationary point is

$$\begin{aligned} \mathbf{x}_s &= -\tfrac{1}{2}\mathbf{B}^{-1}\mathbf{b} \\ &= -\tfrac{1}{2}\begin{bmatrix} -0.7345 & -0.0917 \\ -0.0917 & -1.0096 \end{bmatrix}\begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} = \begin{bmatrix} 0.389 \\ 0.306 \end{bmatrix} \end{aligned}$$



(*a*) The contour plot



(*b*) The response surface plot

Figure 11-11 Contour and response surface plots of the yield response, Example 11-2.

That is, $x_{1,s} = 0.389$ and $x_{2,s} = 0.306$. In terms of the natural variables, the stationary point is

$$0.389 = \frac{\xi_1 - 85}{5} \qquad 0.306 = \frac{\xi_2 - 175}{5}$$

which yields $\xi_1 = 86.95 \simeq 87$ minutes of reaction time and $\xi_2 = 176.53 \simeq 176.5°\text{F}$. This is very close to the stationary point found by visual examination of the contour plot in Figure 11-11. Using Equation 11-8, we may find the predicted response at the stationary point as $\hat{y}_s = 80.21$.

We may also use the canonical analysis described in this section to characterize the response surface. First, it is necessary to express the fitted model in canonical form (Equation 11-9). The eigenvalues λ_1 and λ_2 are the roots of the determinantal equation

$$|\mathbf{B} - \lambda\mathbf{I}| = 0$$

$$\begin{vmatrix} -1.376 - \lambda & 0.1250 \\ 0.1250 & -1.001 - \lambda \end{vmatrix} = 0$$

which reduces to

$$\lambda^2 + 2.3788\lambda + 1.3639 = 0$$

The roots of this quadratic equation are $\lambda_1 = -0.9641$ and $\lambda_2 = -1.4147$. Thus, the canonical form of the fitted model is

$$\hat{y} = 80.21 - 0.9641w_1^2 - 1.4147w_2^2$$

Because both λ_1 and λ_2 are negative and the stationary point is within the region of exploration, we conclude that the stationary point is a maximum.

.....

In some RSM problems it may be necessary to find the relationship between the **canonical variables** $\{w_i\}$ and the **design variables** $\{x_i\}$. This is particularly true if it is impossible to operate the process at the stationary point. As an illustration, suppose that in Example 11-2 we could not operate the process at $\xi_1 = 87$ minutes and $\xi_2 = 176.5°\text{F}$ because this combination of factors results in excessive cost. We now wish to "back away" from the stationary point to a point of lower cost without incurring large losses in yield. The canonical form of the model indicates that the surface is less sensitive to yield loss in the w_1 direction. Exploration of the canonical form requires converting points in the (w_1, w_2) space to points in the (x_1, x_2) space.

In general, the variables $\mathbf{x}$ are related to the canonical variables $\mathbf{w}$ by

$$\mathbf{w} = \mathbf{M}'(\mathbf{x} - \mathbf{x}_s)$$

where $\mathbf{M}$ is a $(k \times k)$ orthogonal matrix. The columns of $\mathbf{M}$ are the normalized eigenvectors associated with the $\{\lambda_i\}$. That is, if $\mathbf{m}_i$ is the ith column of $\mathbf{M}$, then $\mathbf{m}_i$ is the solution to

$$(\mathbf{B} - \lambda_i\mathbf{I})\mathbf{m}_i = \mathbf{0} \tag{11-10}$$

for which $\Sigma_{j=1}^{k} m_{ji}^2 = 1$.

We illustrate the procedure using the fitted second-order model in Example 11-2. For $\lambda_1 = -0.9641$, Equation 11-10 becomes

$$\begin{bmatrix} (-1.376 + 0.9641) & 0.1250 \\ 0.1250 & (-1.001 + 0.9641) \end{bmatrix} \begin{bmatrix} m_{11} \\ m_{21} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

or

$$\begin{aligned} -0.4129m_{11} + 0.1250m_{21} &= 0 \\ 0.1250m_{11} - 0.0377m_{21} &= 0 \end{aligned}$$

We wish to obtain the normalized solution to these equations, that is, the one for which $m_{11}^2 + m_{21}^2 = 1$. There is no unique solution to these equations, so it is most convenient to assign an arbitrary value to one unknown, solve the system, and normalize the solution.

Letting $m_{21}^* = 1$, we find $m_{11}^* = 0.3027$. To normalize this solution, we divide m_{11}^* and m_{21}^* by

$$\sqrt{(m_{11}^*)^2 + (m_{21}^*)^2} = \sqrt{(0.3027)^2 + (1)^2} = 1.0448$$

This yields the normalized solution

$$m_{11} = \frac{m_{11}^*}{1.0448} = \frac{0.3027}{1.0448} = 0.2897$$

and

$$m_{21} = \frac{m_{21}^*}{1.0448} = \frac{1}{1.0448} = 0.9571$$

which is the first column of the **M** matrix.

Using $\lambda_2 = -1.4147$, we can repeat the above procedure, obtaining $m_{12} = -0.9574$ and $m_{22} = 0.2888$ as the second column of **M**. Thus, we have

$$\mathbf{M} = \begin{bmatrix} 0.2897 & -0.9574 \\ 0.9571 & 0.2888 \end{bmatrix}$$

The relationship between the **w** and **x** variables is

$$\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 0.2897 & 0.9571 \\ -0.9574 & 0.2888 \end{bmatrix} \begin{bmatrix} x_1 - 0.389 \\ x_2 - 0.306 \end{bmatrix}$$

or

$$w_1 = 0.2897(x_1 - 0.389) + 0.9571(x_2 - 0.306)$$
$$w_2 = -0.9574(x_1 - 0.389) + 0.2888(x_2 - 0.306)$$

If we wished to explore the response surface in the vicinity of the stationary point, we could determine appropriate points at which to take observations in the (w_1, w_2) space and then use the above relationship to convert these points into the (x_1, x_2) space so that the runs may be made.

11-3.3 Ridge Systems

It is not unusual to encounter variations of the pure maximum, minimum, or saddle point response surfaces discussed in the previous section. Ridge systems, in particular, are fairly common. Consider the canonical form of the second-order model given previously in Equation 11-9:

$$\hat{y} = \hat{y}_s + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \cdots + \lambda_k w_k^2$$

Now suppose that the stationary point $\mathbf{x}_s$ is within the region of experimentation; furthermore, let one or more of the λ_i be very small (e.g., $\lambda_i \simeq 0$). The response variable is then very insensitive to the variables w_i multiplied by the small λ_i.

A contour plot illustrating this situation is shown in Figure 11-12 (page 448) for $k = 2$ variables with $\lambda_1 = 0$. (In practice, λ_1 would be close to but not exactly equal to zero.) The canonical model for this response surface is theoretically

$$\hat{y} = \hat{y}_s + \lambda_2 w_2^2$$

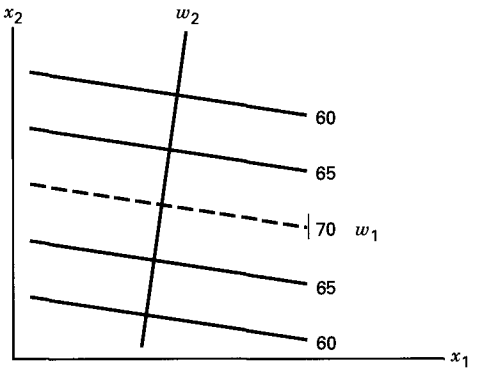


Figure 11-12 A contour plot of a stationary ridge system.

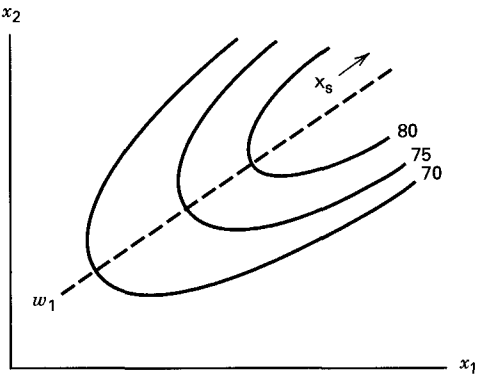


Figure 11-13 A contour plot of a rising ridge system.

with λ_2 negative. Notice that the severe elongation in the w_1 direction has resulted in a line of centers at $\hat{y} = 70$ and the optimum may be taken anywhere along that line. This type of response surface is called a **stationary ridge system.**

If the stationary point is far outside the region of exploration for fitting the second-order model and one (or more) λ_i is near zero, then the surface may be a **rising ridge.** Figure 11-13 illustrates a rising ridge for $k = 2$ variables with λ_1 near zero and λ_2 negative. In this type of ridge system, we cannot draw inferences about the true surface or the stationary point because $\mathbf{x}_s$ is outside the region where we have fit the model. However, further exploration is warranted in the w_1 direction. If λ_2 had been positive, we would call this system a falling ridge.

11-3.4 Multiple Responses

Many response surface problems involve the analysis of several responses. For instance, in Example 11-2, three responses were measured by the experimenter. In that example, we optimized the process with respect to only the yield response y_1.

Simultaneous consideration of multiple responses involves first building an appropriate response surface model for each response and then trying to find a set of operating conditions that in some sense optimizes all responses or at least keeps them in desired ranges. An extensive treatment of the multiple response problem is given in Myers and Montgomery (1995).

We may obtain models for the viscosity and molecular weight responses (y_2 and y_3, respectively) in Example 11-2 as follows:

$$\hat{y}_2 = 70.00 - 0.16x_1 - 0.95x_2 - 0.69x_1^2 - 6.69x_2^2 - 1.25x_1x_2$$
$$\hat{y}_3 = 3386.2 + 205.1x_1 + 17.4x_2$$

In terms of the natural levels of time (ξ_1) and temperature (ξ_2), these models are

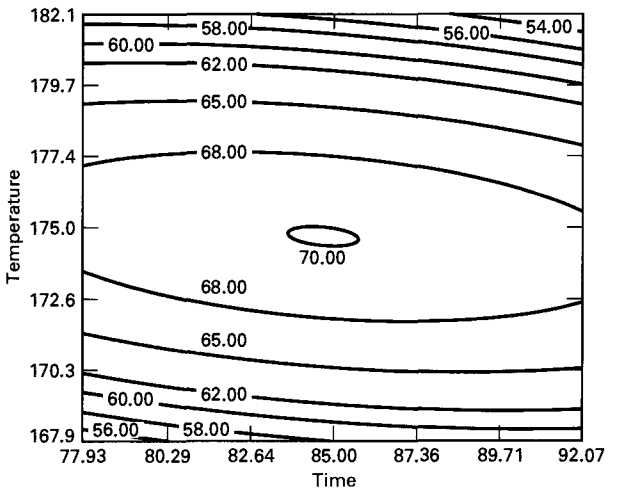
$$\hat{y}_2 = -9030.74 + 13.393\xi_1 + 97.708\xi_2 - 2.75 \times 10^{-2}\xi_1^2 - 0.26757\xi_2^2 - 5 \times 10^{-2}\xi_1\xi_2$$

and

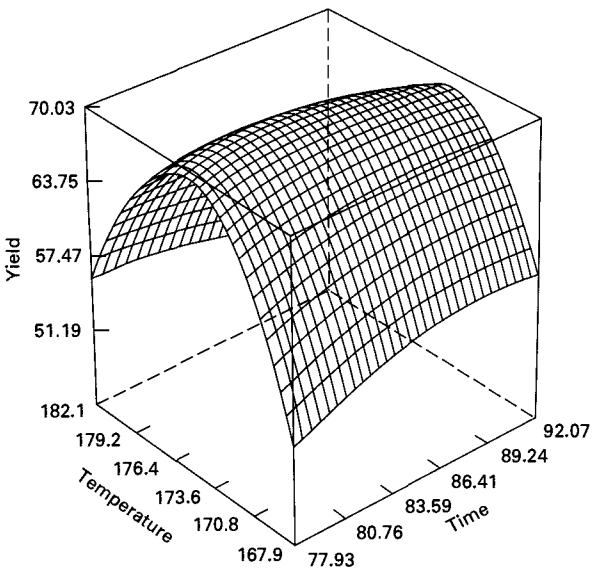
$$\hat{y}_3 = -6308.8 + 41.025\xi_1 + 35.473\xi_2$$

Figures 11-14 and 11-15 (page 450) present the contour and response surface plots for these models.

A relatively straightforward approach to optimizing several responses that works well when there are only a few process variables is to **overlay the contour plots** for each response. Figure 11-16 (page 451) shows an overlay plot for the three responses in Example 11-2, with contours for which y_1 (yield) ≥ 78.5, $62 \leq y_2$ (viscosity) ≤ 68, and y_3 (molecular weight Mn) ≤ 3400. If these boundaries represent important conditions that must be met by the process, then as the unshaded portion of Figure 11-16 shows, there are a number of combinations of time and temperature that will result in a satis-

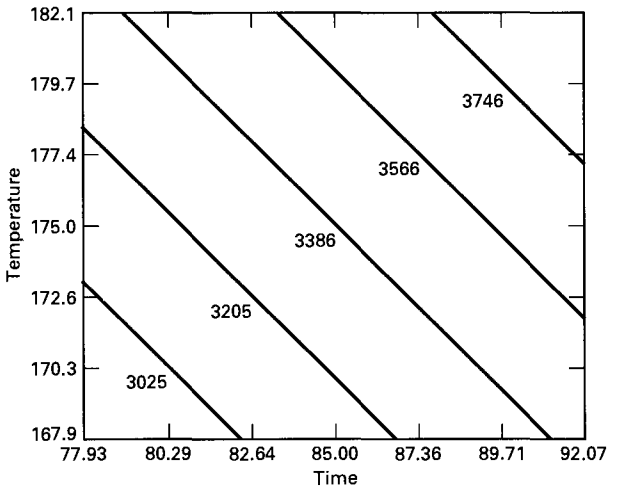


(*a*) The contour plot

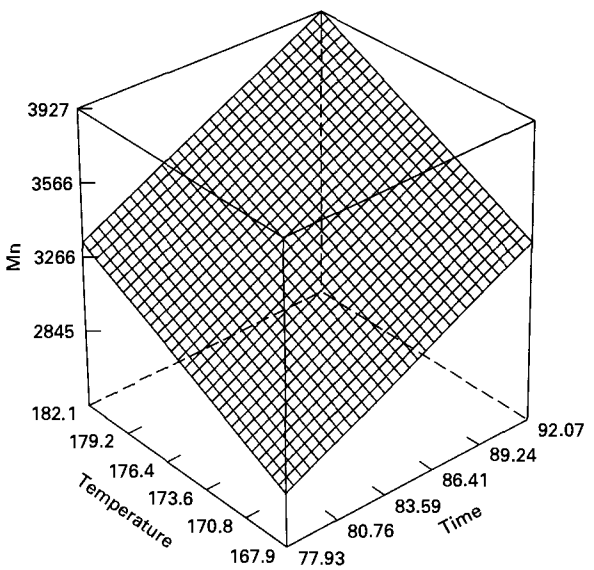


(*b*) The response surface plot

Figure 11-14 Contour plot and response surface plot of viscosity, Example 11-2.



(*a*) The contour plot



(*b*) The response surface plot

Figure 11-15 Contour plot and response surface plot of molecular weight, Example 11-2.

factory process. The experimenter can visually examine the contour plot to determine appropriate operating conditions. For example, it is likely that the experimenter would be most interested in the larger of the two feasible operating regions shown in Figure 11-16.

When there are more than three design variables, overlaying contour plots becomes awkward, because the contour plot is two-dimensional, and $k - 2$ of the design variables must be held constant to construct the graph. Often a lot of trial and error is required to determine which factors to hold constant and what levels to select to obtain the best view of the surface. Therefore, there is practical interest in more formal optimization methods for multiple responses.

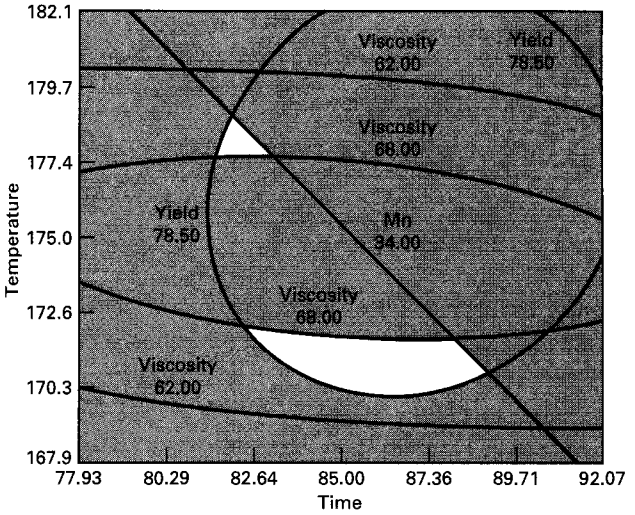


Figure 11-16 Region of the optimum found by overlaying yield, viscosity, and molecular weight response surfaces, Example 11-2.

A popular approach is to formulate and solve the problem as a **constrained optimization problem**. To illustrate using Example 11-2, we might formulate the problem as

$$\begin{gathered}\text{Max } y_1 \\ \text{subject to} \\ 62 \leq y_2 \leq 68 \\ y_3 \leq 3400\end{gathered}$$

There are many numerical techniques that can be used to solve this problem. Sometimes these techniques are referred to as **nonlinear programming methods**. The Design-Expert software package solves this version of the problem using a direct search procedure. The two solutions found are

$$\text{time} = 83.5 \qquad \text{temp} = 177.1 \qquad \hat{y}_1 = 79.5$$

and

$$\text{time} = 86.6 \qquad \text{temp} = 172.25 \qquad \hat{y}_1 = 79.5$$

Notice that the first solution is in the upper (smaller) feasible region of the design space (refer to Figure 11-16), whereas the second solution is in the larger region. Both solutions are very near to the boundary of the constraints.

Another useful approach to optimization of multiple responses is to use the simultaneous optimization technique popularized by Derringer and Suich (1980). Their procedure makes use of **desirability functions**. The general approach is to first convert each response y_i into an individual desirability function d_i that varies over the range

$$0 \leq d_i \leq 1$$

where if the response y_i is at its goal or target, then $d_i = 1$, and if the response is outside an acceptable region, $d_i = 0$. Then the design variables are chosen to maximize the overall desirability

$$D = (d_1 \cdot d_2 \cdot \cdots \cdot d_m)^{1/m}$$

where there are m responses.

The individual desirability functions are structured as shown in Figure 11-17 on the facing page. If the objective or target T for the response y is a maximum value,

$$d = \begin{cases} 0 & y < L \\ \left(\dfrac{y - L}{T - L}\right)^r & L \leq y \leq T \\ 1, & y > T \end{cases} \tag{11-11}$$

when the weight $r = 1$, the desirability function is linear. Choosing $r > 1$ places more emphasis on being close to the target value, and choosing $0 < r < 1$ makes this less important. If the target for the response is a minimum value,

$$d = \begin{cases} 1 & y < T \\ \left(\dfrac{U - y}{U - T}\right)^r & T \leq y \leq U \\ 0 & y > U \end{cases} \tag{11-12}$$

The two-sided desirability function shown in Figure 11-17(c) assumes that the target is located between the lower (L) and upper (U) limits, and is defined as

$$d = \begin{cases} 0 & y < L \\ \left(\dfrac{y - L}{T - L}\right)^{r_1} & L \leq y \leq T \\ \left(\dfrac{U - y}{U - T}\right)^{r_2} & T \leq y \leq U \\ 0 & y > U \end{cases} \tag{11-13}$$

The Design-Expert software package was used to solve Example 11-2 using the desirability function approach. We chose $T = 80$ as the target for the yield response, $L = 70$, and set the weight for this individual desirability equal to unity. We set $T = 65$ for the viscosity response with $L = 62$ and $U = 68$ (to be consistent with specifications), with both weights $r_1 = r_2 = 1$. Finally, we indicated that any molecular weight between 3200 and 3400 was acceptable. Two solutions were found.

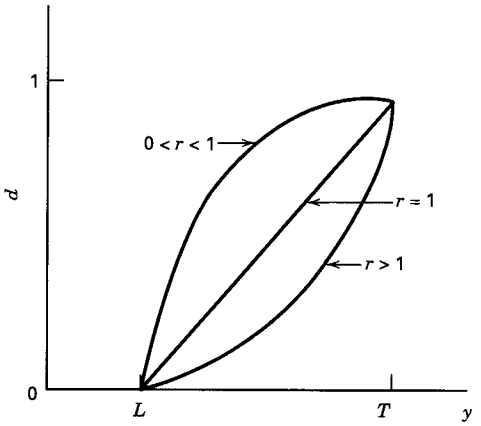
Solution 1:

Time = 86.5	Temp = 170.5	$D = 0.822$
$\hat{y}_1 = 78.8$	$\hat{y}_2 = 65$	$\hat{y}_3 = 3287$

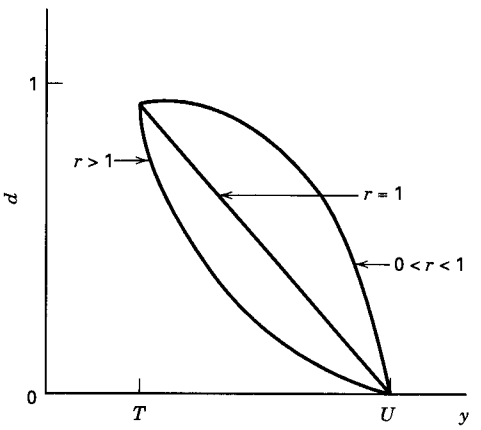
Solution 2:

Time = 82	Temp = 178.8	$D = 0.792$
$\hat{y}_1 = 78.5$	$\hat{y}_2 = 65$	$\hat{y}_3 = 3400$

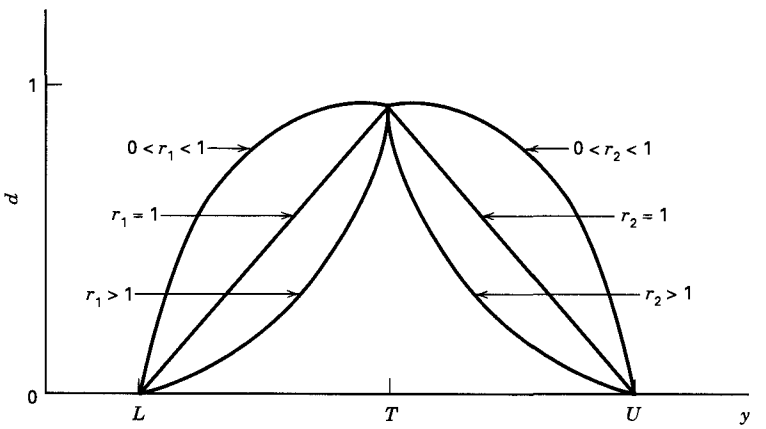
Solution 1 has the highest overall desirability. Notice that it results in on-target viscosity and acceptable molecular weight. This solution is in the larger of the two operating regions in Figure 11-16, whereas the second solution is in the smaller region. Figure 11-18 (page 454) shows a response and contour plot of the overall desirability function D.



(a) Objective (target) is to maximize y



(b) Objective (target) is to minimize y



(c) Objective is for y to be as close as posible to the target

Figure 11-17 Individual desirability functions for simultaneous optimization.

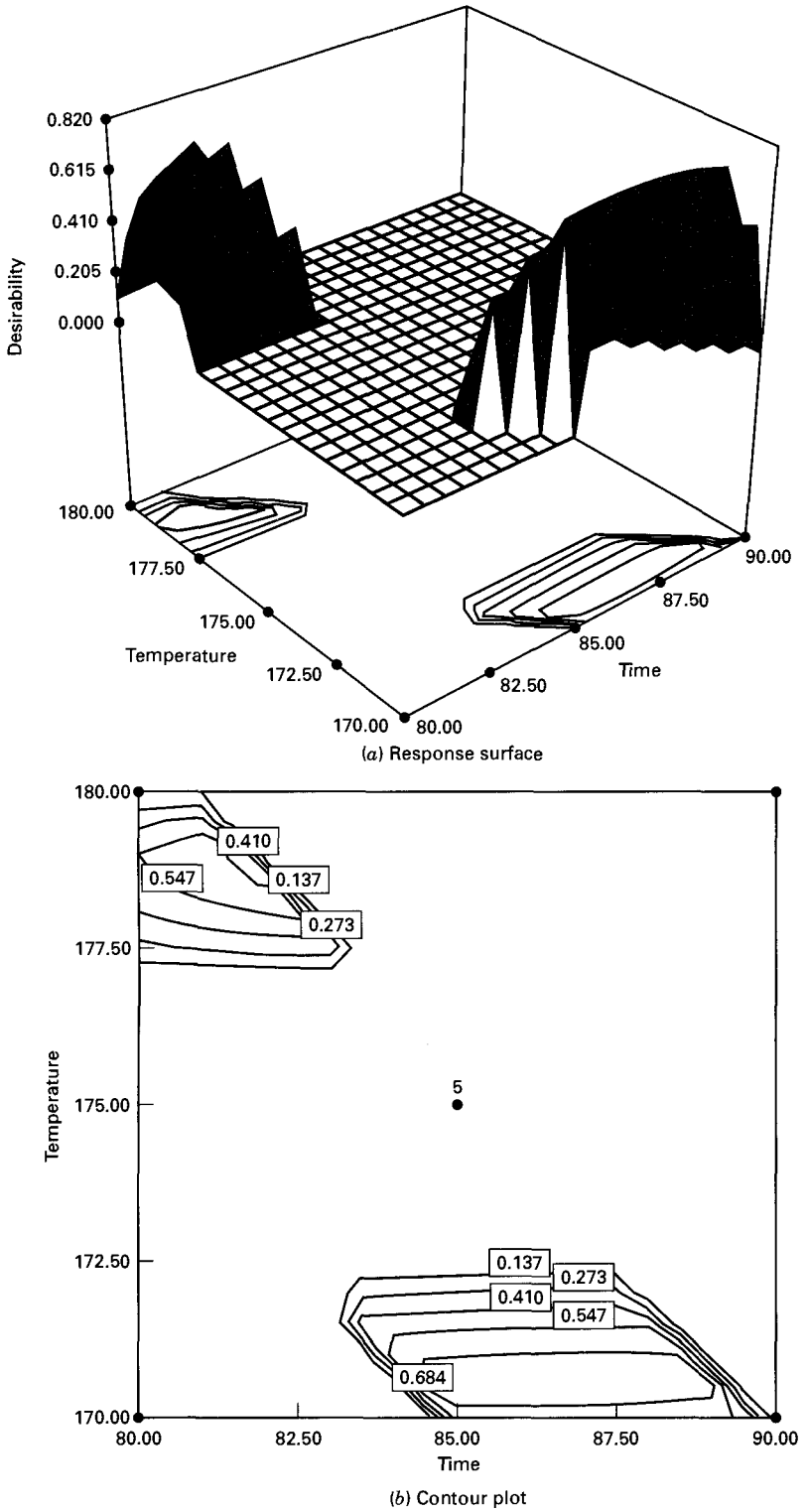


Figure 11-18 Desirability function response surface and contour plot for the problem in Example 11-2.

11-4 EXPERIMENTAL DESIGNS FOR FITTING RESPONSE SURFACES

Fitting and analyzing response surfaces is greatly facilitated by the proper choice of an experimental design. In this section, we discuss some aspects of selecting appropriate designs for fitting response surfaces.

When selecting a response surface design, some of the features of a desirable design are as follows:

1. Provides a reasonable distribution of data points (and hence information) throughout the region of interest
2. Allows model adequacy, including lack of fit, to be investigated
3. Allows experiments to be performed in blocks
4. Allows designs of higher order to be built up sequentially
5. Provides an internal estimate of error
6. Provides precise estimates of the model coefficients
7. Provides a good profile of the prediction variance throughout the experimental region
8. Provides reasonable robustness against outliers or missing values
9. Does not require a large number of runs
10. Does not require too many levels of the independent variables
11. Ensures simplicity of calculation of the model parameters

These features are sometimes conflicting, so judgment must often be applied in design selection. For more information on the choice of a response surface design, refer to Myers and Montgomery (1995), Box and Draper (1987), and Khuri and Cornell (1996).

11-4.1 Designs for Fitting the First-Order Model

Suppose we wish to fit the first-order model in k variables

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \epsilon \tag{11-14}$$

There is a unique class of designs that minimize the variance of the regression coefficients $\{\hat{\beta}_i\}$. These are the **orthogonal first-order designs**. A first-order design is orthogonal if the off-diagonal elements of the $(\mathbf{X}'\mathbf{X})$ matrix are all zero. This implies that the cross-products of the columns of the $\mathbf{X}$ matrix sum to zero.

The class of orthogonal first-order designs includes the 2^k factorial and fractions of the 2^k series in which main effects are not aliased with each other. In using these designs, we assume that the low and high levels of the k factors are coded to the usual ± 1 levels.

The 2^k design does not afford an estimate of the experimental error unless some runs are replicated. A common method of including replication in the 2^k design is to augment the design with several observations at the center (the point $x_i = 0, i = 1, 2, \ldots, k$). The addition of center points to the 2^k design does not influence the $\{\hat{\beta}_i\}$ for $i \geq 1$, but the estimate of β_0 becomes the grand average of all observations. Furthermore, the addition of center points does not alter the orthogonality property of the design. Example 11-1

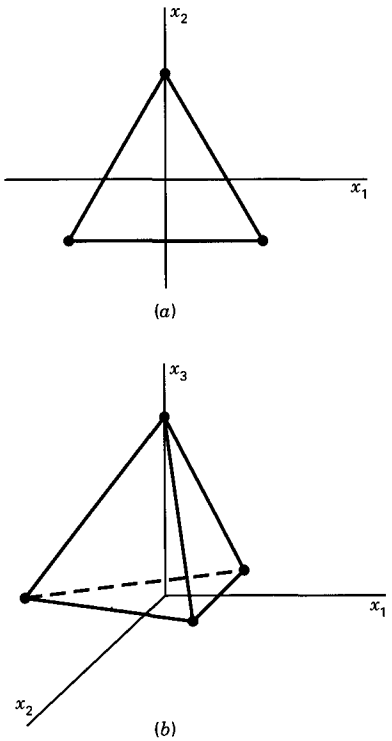


Figure 11-19 The simplex design for (*a*) $k = 2$ variables and (*b*) $k = 3$ variables.

illustrates the use of a 2^2 design augmented with five center points to fit a first-order model.

Another orthogonal first-order design is the **simplex**. The simplex is a regularly sided figure with $k + 1$ vertices in k dimensions. Thus, for $k = 2$ the simplex design is an equilateral triangle and for $k = 3$ it is a regular tetrahedron. Simplex designs in two and three dimensions are shown in Figure 11-19.

11-4.2 Designs for Fitting the Second-Order Model

We have informally introduced in Example 11-2 (and even earlier, in Example 6-6) the **central composite design** or **CCD** for fitting a second-order model. This is the most popular class of designs used for fitting these models. Generally, the CCD consists of a 2^k factorial (or fractional factorial of resolution V) with n_F runs, $2k$ axial or star runs, and n_C center runs. Figure 11-20 (on the facing page) shows the CCD for $k = 2$ and $k = 3$ factors.

The practical deployment of a CCD often arises through **sequential experimentation**, as in Examples 11-1 and 11-2. That is, a 2^k has been used to fit a first-order model, this model has exhibited lack of fit, and the axial runs are then added to allow the quadratic terms to be incorporated into the model. The CCD is a very efficient design for fitting the second-order model. There are two parameters in the design that must be specified: the distance α of the axial runs from the design center and the number of center points n_C. We now discuss the choice of these two parameters.

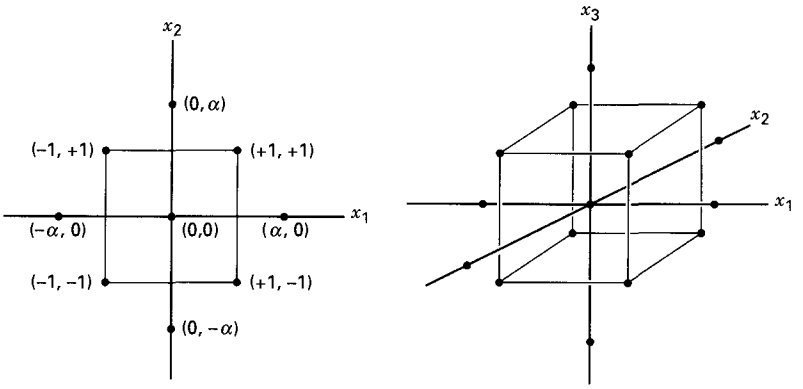


Figure 11-20 Central composite designs for $k = 2$ and $k = 3$.

Rotatability

It is important for the second-order model to provide good predictions throughout the region of interest. One way to define "good" is to require that the model have a reasonably consistent and stable variance of the predicted response at points of interest **x**. Recall Equation 10-40 that the variance of the predicted response at some point **x** is

$$V[\hat{y}(\mathbf{x})] = \sigma^2 \mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}$$

Box and Hunter (1957) suggested that a second-order response surface design should be **rotatable**. This means that the $V[\hat{y}(\mathbf{x})]$ is the same at all points **x** that are the same distance from the design center. That is, the variance of predicted response is constant on spheres.

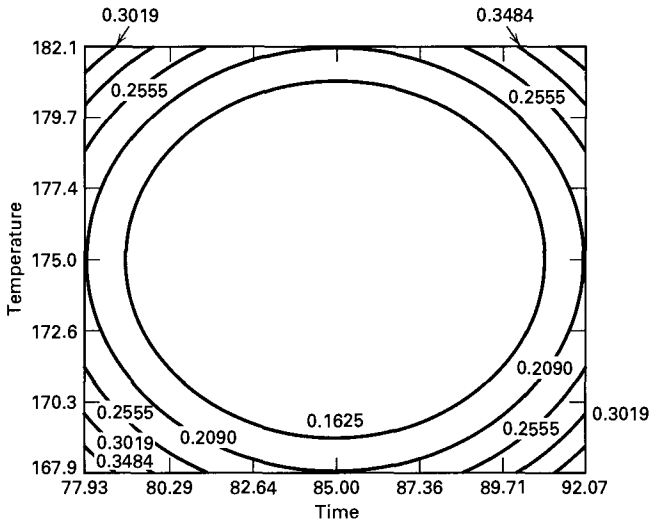
Figure 11-21 (page 458) shows contours of constant $\sqrt{V[\hat{y}(\mathbf{x})]}$ for the second-order model fit using the CCD in Example 11-2. Notice that the contours of constant standard deviation of predicted response are concentric circles. A design with this property will leave the variance of $\hat{y}$ unchanged when the design is rotated about the center $(0, 0, \ldots, 0)$, hence, the name *rotatable* design.

Rotatability is a reasonable basis for the selection of a response surface design. Because the purpose of RSM is optimization and the location of the optimum is unknown prior to running the experiment, it makes sense to use a design that provides equal precision of estimation in all directions (it can be shown that any first-order orthogonal design is rotatable).

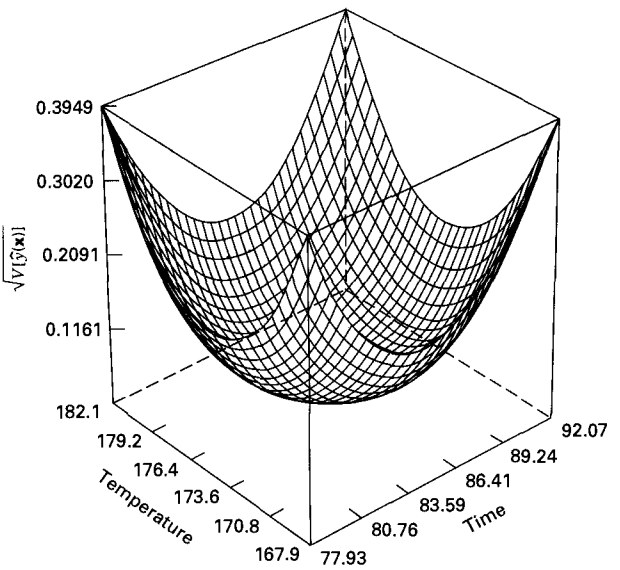
A central composite design is made rotatable by the choice of α. The value of α for rotatability depends on the number of points in the factorial portion of the design; in fact, $\alpha = (n_F)^{1/4}$ yields a rotatable central composite design where n_F is the number of points used in the factorial portion of the design.

The Spherical CCD

Rotatability is a spherical property; that is, it makes the most sense as a design criterion when the region of interest is a sphere. However, it is not important to have exact rotatability to have a good design. In fact, for a spherical region of interest, the best choice of α from a prediction variance viewpoint for the CCD is to set $\alpha = \sqrt{k}$. This design, called a **spherical CCD**, puts all the factorial and axial design points on the surface of a sphere of radius $\sqrt{k}$. For more discussion of this, see Myers and Montgomery (1995).



(*a*) Contours of $\sqrt{V[\hat{y}(\mathbf{x})]}$



(*b*) The response surface plot

Figure 11-21 Contours of constant standard deviation of predicted response for the rotatable CCD, Example 11-2.

Center Runs in the CCD

The choice of α in the CCD is dictated primarily by the region of interest. When this region is a sphere, the design must include center runs to provide reasonably stable variance of predicted response. Generally, three to five center runs are recommended.

The Box–Behnken Design

Box and Behnken (1960) have proposed some three-level designs for fitting response surfaces. These designs are formed by combining 2^k factorials with incomplete block

Table 11-8 A Three-Variable Box–Behnken Design

Run	x_1	x_2	x_3
1	−1	−1	0
2	−1	1	0
3	1	−1	0
4	1	1	0
5	−1	0	−1
6	−1	0	1
7	1	0	−1
8	1	0	1
9	0	−1	−1
10	0	−1	1
11	0	1	−1
12	0	1	1
13	0	0	0
14	0	0	0
15	0	0	0

designs. The resulting designs are usually very efficient in terms of the number of required runs, and they are either rotatable or nearly rotatable.

Table 11-8 shows a three-variable Box–Behnken design. The design is also shown geometrically in Figure 11-22. Notice that the Box–Behnken design is a spherical design, with all points lying on a sphere of radius $\sqrt{2}$. Also, the Box–Behnken design does not contain any points at the vertices of the cubic region created by the upper and lower limits for each variable. This could be advantageous when the points on the corners of the cube represent factor-level combinations that are prohibitively expensive or impossible to test because of physical process constraints.

Cuboidal Region of Interest

There are many situations where the region of interest is cuboidal rather than spherical. In these cases, a useful variation of the central composite design is the **face-centered central composite design** or the **face-centered cube**, in which $\alpha = 1$. This design locates the star or axial points on the centers of the faces of the cube, as shown in Figure 11-23 for $k = 3$. This variation of the central composite design is also sometimes used because it requires only three levels of each factor, and in practice it is frequently difficult to

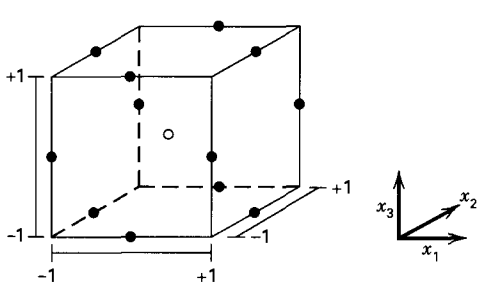


Figure 11-22 A Box–Behnken design for three factors.

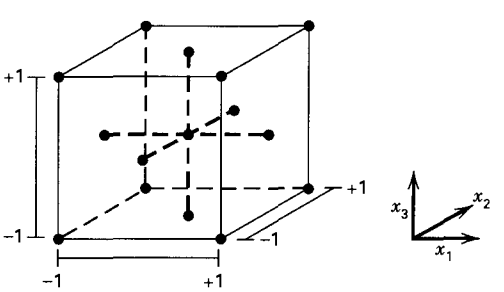
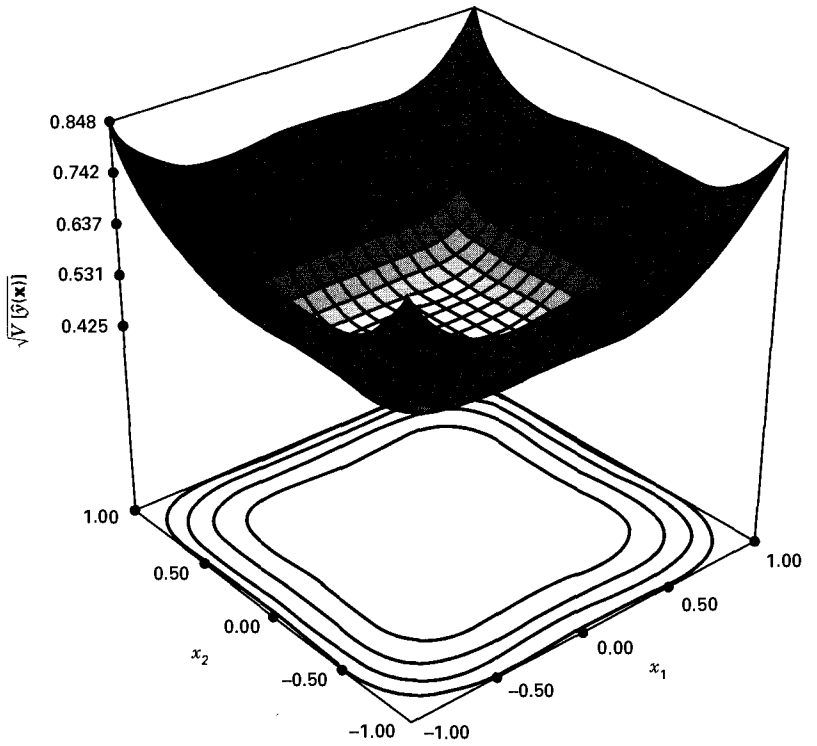
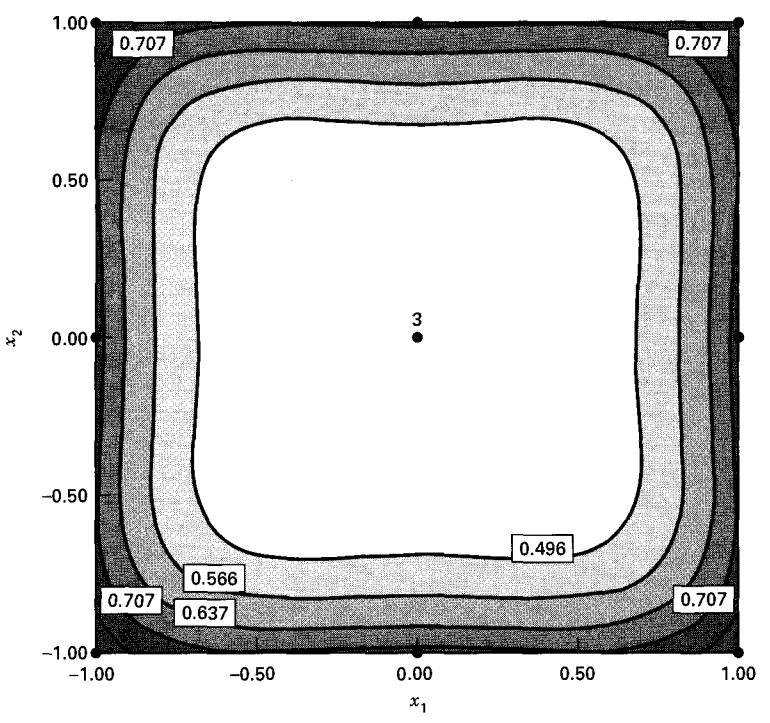


Figure 11-23 A face-centered central composite design for $k = 3$.



(*a*) Response surface



(*b*) Contour plot

Figure 11-24 Standard deviation of predicted response $\sqrt{V[\hat{y}(\mathbf{x})]}$ for the face-centered cube with $k = 3$, $n_C = 3$, and $x_3 = 0$.

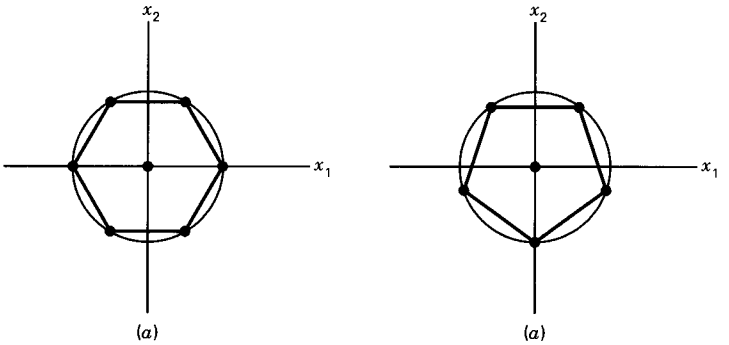


Figure 11-25 Equiradial designs for two variables. (*a*) Hexagon. (*b*) Pentagon.

change factor levels. However, note that face-centered central composite designs are not rotatable.

The face-centered cube does not require as many center points as the spherical CCD. In practice, $n_C = 2$ or 3 is sufficient to provide good variance of prediction throughout the experimental region. It should be noted that sometimes more center runs will be employed to give a reasonable estimate of experimental error. Figure 11-24 (on the facing page) shows the square root of prediction variance $\sqrt{V[\hat{y}(\mathbf{x})]}$ for the face-centered cube for $k = 3$ with $n_C = 3$ center points ($x_3 = 0$). Notice that the standard deviation of predicted response is reasonably uniform over a relatively large portion of the design space.

Other Designs

There are many other response surface designs that are occasionally useful in practice. For two variables, we could use designs consisting of points that are equally spaced on a circle and that form regular polygons. Because the design points are equidistant from the origin, these arrangements are often called **equiradial designs.**

For $k = 2$, a rotatable equiradial design is obtained by combining $n_2 \geq 5$ points equally spaced on a circle with $n_1 \geq 1$ points at the center of the circle. Particularly useful designs for $k = 2$ are the pentagon and hexagon. These designs are shown in Figure 11-25. Other useful designs include the **small composite design**, consisting of a fractional factorial in the cube of resolution III* (main effects aliased with two-factor interactions and no two-factor interactions aliased with each other) and the usual axial and center runs, and the class of **hybrid designs**. Both of these designs may be of considerable value when it is important to reduce the number of runs as much as possible.

A small composite design for $k = 3$ factors is shown in Table 11-9 (on the next page). This design uses the standard one-half fraction of the 2^3 in the cube because it meets the resolution III* criteria. The design has four runs in the cube and six axial runs, and it must have at least one center point. Thus the design has a minimum of $N = 11$ trials, and the second-order model in $k = 3$ variables has $p = 10$ parameters to estimate, so this is a very efficient design with respect to the number of runs. The design in Table 11-9 has $n_C = 4$ center runs. We selected $\alpha = 1.73$ to give a spherical design because the small composite design cannot be made rotatable.

A hybrid design for $k = 3$ is shown in Table 11-10 on the next page. Some of these designs have irregular levels, and this can be a limiting factor in their application. How-

Table 11-9 A Small Composite Design for $k = 3$ Factors

Standard Order	x_1	x_2	x_3
1	1.00	1.00	−1.00
2	1.00	−1.00	1.00
3	−1.00	1.00	1.00
4	−1.00	−1.00	−1.00
5	−1.73	0.00	0.00
6	1.73	0.00	0.00
7	0.00	−1.73	0.00
8	0.00	1.73	0.00
9	0.00	0.00	−1.73
10	0.00	0.00	1.73
11	0.00	0.00	0.00
12	0.00	0.00	0.00
13	0.00	0.00	0.00
14	0.00	0.00	0.00

ever, they are very small designs, and they have excellent prediction variance properties. For more details about small composite designs and hybrid designs, refer to Myers and Montgomery (1995).

11-4.3 Blocking in Response Surface Designs

When using response surface designs, it is often necessary to consider blocking to eliminate nuisance variables. For example, this problem may occur when a second-order design is assembled sequentially from a first-order design, as was illustrated in Examples 11-1 and 11-2. Considerable time may elapse between the running of the first-order

Table 11-10 A Hybrid Design for $k = 3$ Factors

Standard Order	x_1	x_2	x_3
1	0.00	0.00	1.41
2	0.00	0.00	−1.41
3	−1.00	−1.00	0.71
4	1.00	−1.00	0.71
5	−1.00	1.00	0.71
6	1.00	1.00	0.71
7	1.41	0.00	−0.71
8	−1.41	0.00	−0.71
9	0.00	1.41	−0.71
10	0.00	−1.41	−0.71
11	0.00	0.00	0.00

design and the running of the supplemental experiments required to build up a second-order design, and during this time test conditions may change, thus necessitating blocking.

A response surface design is said to **block orthogonally** if it is divided into blocks such that block effects do not affect the parameter estimates of the response surface model. If a 2^k or 2^{k-p} design is used as a first-order response surface design, the methods of Chapter 7 may be used to arrange the runs in 2^r blocks. The center points in these designs should be allocated equally among the blocks.

For a second-order design to block orthogonally, two conditions must be satisfied. If there are n_b observations in the bth block, then these conditions are

1. Each block must be a first-order orthogonal design; that is,

$$\sum_{u=1}^{n_b} x_{iu}x_{ju} = 0 \qquad i \neq j = 0, 1, \ldots, k \qquad \text{for all } b$$

where x_{iu} and x_{ju} are the levels of ith and jth variables in the uth run of the experiment with $x_{0u} = 1$ for all u.

2. The fraction of the total sum of squares for each variable contributed by every block must be equal to the fraction of the total observations that occur in the block; that is,

$$\frac{\sum_{u=1}^{n_b} x_{iu}^2}{\sum_{u=1}^{N} x_{iu}^2} = \frac{n_b}{N} \qquad i = 1, 2, \ldots, k \qquad \text{for all } b$$

where N is the number of runs in the design.

As an example of applying these conditions, consider a rotatable central composite design in $k = 2$ variables with $N = 12$ runs. We may write the levels of x_1 and x_2 for this design in the design matrix

$$\mathbf{D} = \begin{array}{c} \\ \left[\begin{array}{cc} x_1 & x_2 \\ -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \\ 0 & 0 \\ 0 & 0 \\ 1.414 & 0 \\ -1.414 & 0 \\ 0 & 1.414 \\ 0 & -1.414 \\ 0 & 0 \\ 0 & 0 \end{array}\right] \end{array} \begin{array}{l} \\ \left.\begin{array}{l} \\ \\ \\ \\ \\ \\ \end{array}\right\} \text{Block 1} \\ \left.\begin{array}{l} \\ \\ \\ \\ \\ \\ \end{array}\right\} \text{Block 2} \end{array}$$

Notice that the design has been arranged in two blocks, with the first block consisting of the factorial portion of the design plus two center points and the second block con-

sisting of the axial points plus two additional center points. It is clear that condition 1 is met; that is, both blocks are first-order orthogonal designs. To investigate condition two, consider first block 1 and note that

$$\sum_{u=1}^{n_1} x_{1u}^2 = \sum_{u=1}^{n_1} x_{2u}^2 = 4$$

$$\sum_{u=1}^{N} x_{1u}^2 = \sum_{u=1}^{N} x_{2u}^2 = 8 \qquad \text{and} \qquad n_1 = 6$$

Therefore,

$$\frac{\sum_{u=1}^{n_1} x_{iu}^2}{\sum_{u=1}^{N} x_{iu}^2} = \frac{n_1}{N}$$

$$\frac{4}{8} = \frac{6}{12}$$

Thus, condition 2 is satisfied in block 1. For block 2, we have

$$\sum_{u=1}^{n_2} x_{1u}^2 = \sum_{u=1}^{n_2} x_{2u}^2 = 4 \qquad \text{and} \qquad n_2 = 6$$

Therefore,

$$\frac{\sum_{u=1}^{n_2} x_{iu}^2}{\sum_{u=1}^{N} x_{iu}^2} = \frac{n_2}{N}$$

$$\frac{4}{8} = \frac{6}{12}$$

Because condition 2 is also satisfied in block 2, this design blocks orthogonally.

In general, the central composite design can always be constructed to block orthogonally in two blocks with the first block consisting of n_F factorial points plus n_{CF} center points and the second block consisting of $n_A = 2k$ axial points plus n_{CA} center points. The first condition for orthogonal blocking will always hold regardless of the value used for α in the design. For the second condition to hold,

$$\frac{\sum_{u}^{n_2} x_{iu}^2}{\sum_{u}^{n_1} x_{iu}^2} = \frac{n_A + n_{CA}}{n_F + n_{CF}} \tag{11-15}$$

The left-hand side of Equation 11-15 is $2\alpha^2/n_F$, and after substituting in this quantity, we may solve the equation for the value of α that will result in orthogonal blocking as

$$\alpha = \left[\frac{n_F(n_A + n_{CA})}{2(n_F + n_{CF})}\right]^{1/2} \tag{11-16}$$

This value of α does not, in general, result in a rotatable or spherical design. If the design is also required to be rotatable, then $\alpha = (n_F)^{1/4}$ and

$$(n_F)^{1/2} = \frac{n_F(n_A + n_{CA})}{2(n_F + n_{CF})} \tag{11-17}$$

It is not always possible to find a design that exactly satisfies Equation 11-17. For example if $k = 3$, $n_F = 8$ and $n_A = 6$, and Equation 11-17 reduces to

$$(8)^{1/2} = \frac{8(6 + n_{CA})}{2(8 + n_{CF})}$$

$$2.83 = \frac{48 + 8n_{CA}}{16 + 2n_{CF}}$$

It is impossible to find values of n_{CA} and n_{CF} that exactly satisfy this last equation. However, note that if $n_{CF} = 3$ and $n_{CA} = 2$, then the right-hand side is

$$\frac{48 + 8(2)}{16 + 2(3)} = 2.91$$

so the design nearly blocks orthogonally. In practice, one could relax somewhat the requirement of either rotatability or orthogonal blocking without any major loss of information.

The central composite design is very versatile in its ability to accommodate blocking. If k is large enough, the factorial portion of the design can be divided into two or more blocks. (The number of factorial blocks must be a power of 2, with the axial portion forming a single block.) Table 11-11 presents several useful blocking arrangements for the central composite design.

Table 11-11 Some Rotatable and Near-Rotatable Central Composite Designs That Block Orthogonally

k	2	3	4	5	5 $\frac{1}{2}$ Rep.	6	6 $\frac{1}{2}$ Rep.	7	7 $\frac{1}{2}$ Rep.
Factorial Block(s)									
n_F	4	8	16	32	16	64	32	128	64
Number of blocks	1	2	2	4	1	8	2	16	8
Number of points in each block	4	4	8	8	16	8	16	8	8
Number of center points in each block	3	2	2	2	6	1	4	1	1
Total number of points in each block	7	6	10	10	22	9	20	9	9
Axial Block									
n_A	4	6	8	10	10	12	12	14	14
n_{CA}	3	2	2	4	1	6	2	11	4
Total number of points in the axial block	7	8	10	14	11	18	14	25	18
Total number of points N in the design	14	20	30	54	33	90	54	169	80
Values of α									
Orthogonal blocking	1.4142	1.6330	2.0000	2.3664	2.0000	2.8284	2.3664	3.3636	2.8284
Rotatability	1.4142	1.6818	2.0000	2.3784	2.0000	2.8284	2.3784	3.3333	2.8284

There are two important points about the analysis of variance when the response surface design has been run in blocks. The first concerns the use of center points to calculate an estimate of pure error. Only center points that are run in the same block can be considered to be replicates, so the pure error term can only be calculated within each block. If the variability is consistent across blocks, then these pure error estimates could be pooled. The second point concerns the block effect. If the design blocks orthogonally in m blocks, the sum of squares for blocks is

$$SS_{\text{Blocks}} = \sum_{b=1}^{m} \frac{B_b^2}{n_b} - \frac{G^2}{N} \tag{11-18}$$

where B_b is the total of the n_b observations in the bth block and G is the grand total of all N observations in all m blocks. When blocks are not exactly orthogonal, the general regression significance test (the "extra sum of squares" method) described in Chapter 10 can be used.

11-4.4 Computer-Generated (Optimal) Designs

The standard response surface designs discussed in the previous sections, such as the central composite design, the Box–Behnken design, and their variations (such as the face-centered cube) are widely used because they are quite general and flexible designs. If the experimental region is either a cube or a sphere, there is typically a standard response surface design that will be applicable to the problem. However, occasionally an experimenter encounters a situation where a standard response surface design may not be the obvious choice. **Computer-generated** designs are an alternative to consider in these cases.

There are three situations where some type of computer-generated design may be appropriate.

*1. **An irregular experimental region.*** If the region of interest for the experiment is not a cube or a sphere, standard designs may not be the best choice. Irregular regions of interest occur fairly often. For example, an experimenter is investigating the properties of a particular adhesive. The adhesive is applied to two parts and then cured at an elevated temperature. The two factors of interest are the amount of adhesive applied and the cure temperature. Over the ranges of these two factors, taken as -1 to $+1$ on the usual coded variable scale, the experimenter knows that if too little adhesive is applied and the cure temperature is too low, the parts will not bond satisfactorily. In terms of the coded variables, this leads to a **constraint** on the design variables, say

$$-1.5 \leq x_1 + x_2$$

where x_1 represents the application amount of adhesive and x_2 represents the temperature. Furthermore, if the temperature is too high and too much adhesive is applied, the parts will be either damaged by heat stress or an inadequate bond will result. Thus, there is another constraint on the factor levels

$$x_1 + x_2 \leq 1$$

Figure 11-26 (on the next page) shows the experimental region that results from applying these constraints. Notice that the constraints effectively remove two corners of the square, producing an irregular experimental region (sometimes these irregular regions are called

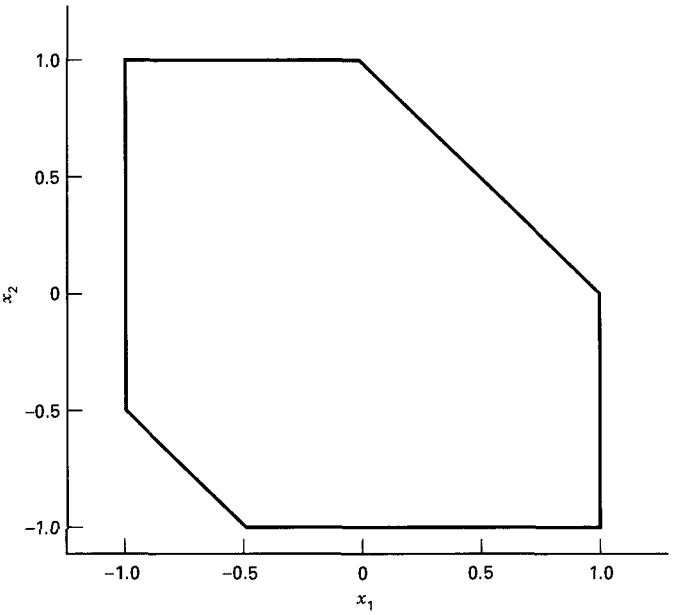


Figure 11-26 A constrained design region in two variables.

"dented cans"). There is no standard response surface design that will fit exactly into this region.

*2. **A nonstandard model.*** Usually an experimenter elects a first- or second-order response surface model, realizing that this **empirical model** is an approximation to the true underlying mechanism. However, sometimes the experimenter may have some special knowledge or insight about the process being studied that may suggest a nonstandard model. For example, the model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{112} x_1^2 x_2 + \beta_{1112} x_1^3 x_2 + \epsilon$$

may be of interest. The experimenter would be interested in obtaining an efficient design for fitting this reduced quartic model. As another illustration, sometimes we encounter response surface problems where some of the design factors are categorical variables. There are no standard response surface designs for this situation [refer to Myers and Montgomery (1995) for a discussion of categorical variables in response surface problems].

*3. **Unusual sample size requirements.*** Occasionally an experimenter may need to reduce the number of runs required by a standard response surface design. For example, suppose we intend to fit a second-order model in four variables. The central composite design for this situation requires between 28 and 30 runs, depending on the number of center points selected. However, the model has only 15 terms. If the runs are extremely expensive or time-consuming, the experimenter will want a design with fewer trials. Although computer-generated designs can be used for this purpose, there are usually better approaches. For example, a small composite design can be constructed for four

factors with 20 runs, including four center points, and a hybrid design with as few as 16 runs is also available. These are generally superior choices to using a computer-generated design to reduce the number of trials.

Much of the development of computer-generated designs is an outgrowth of work by Kiefer (1959, 1961) and Kiefer and Wolfowitz (1959) in the theory of **optimal designs**. By an optimal design, we mean a design that is "best" with respect to some criterion. Computer programs are required to construct these designs. The usual approach is to specify a model, determine the region of interest, select the number of runs to make, specify the optimality criterion, and then choose the design points from a set of *candidate* points that the experimenter would consider using. Typically, the candidate points are a grid of points spaced over the feasible design region.

There are several popular design optimality criteria. Perhaps the most widely used is the D-optimality criterion. A design is said to be **D-optimal** if

$$|(\mathbf{X}'\mathbf{X})^{-1}|$$

is minimized. It turns out that a D-optimal design minimizes the volume of the joint confidence region on the vector of regression coefficients. A measure of the relative efficiency of design 1 to design 2 according to the D-criterion is given by

$$D_e = \left(\frac{|(\mathbf{X}_2'\mathbf{X}_2)^{-1}|}{|(\mathbf{X}_1'\mathbf{X}_1)^{-1}|} \right)^{1/p} \tag{11-19}$$

where $\mathbf{X}_1$ and $\mathbf{X}_2$ are the $\mathbf{X}$ matrices for the two designs and p is the number of model parameters.

The ***A*-optimality** criterion deals with only the variances of the regression coefficients. A design is A-optimal if it minimizes the sum of the main diagonal elements of $(\mathbf{X}'\mathbf{X})^{-1}$ (this is called the **trace** of $(\mathbf{X}'\mathbf{X})^{-1}$, usually denoted $\text{tr}(\mathbf{X}'\mathbf{X})^{-1}$). Thus an A-optimal design minimizes the sum of the variances of the regression coefficients.

Because many response surface experiments are concerned with prediction of the response, **prediction variance criteria** are of considerable practical interest. Perhaps the most popular of these is the ***G*-optimality criterion**. A design is said to be G-optimal if it minimizes the maximum scaled prediction variance over the design region. That is, if the maximum value of

$$\frac{NV[\hat{y}(\mathbf{x})]}{\sigma^2}$$

over the design region is a minimum, where N is the number of points in the design. If the model has p parameters, the G-efficiency of a design is just

$$G_e = \frac{p}{\max \dfrac{NV[\hat{y}(\mathbf{x})]}{\sigma^2}} \tag{11-20}$$

The ***V*-criterion** considers the prediction variance at a *set* of points of interest in the design region, say $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m$. The set of points could be the candidate set from which the design was selected, or it could be some other collection of points that have specific meaning to the experimenter. A design that minimizes the *average* prediction variance over this set of m points is a ***V*-optimal design**.

Collectively, the design criteria that we have been discussing are often called **alphabetic optimality criteria**. There are some situations for which the alphabetically

optimal design is either known or can be constructed analytically. A good example is the 2^k design, which is D-, A-, G-, and V-optimal for fitting the first-order model in k variables or for fitting the first-order model with interaction. However, in most cases, the optimal design is not known and a computer-based algorithm must be employed to find a design. Many statistical software packages that support designed experiments have this capability. Most of the design construction procedures are based on the **exchange algorithm**. Essentially, a grid of candidate points is selected by the experimenter and an initial design is selected (perhaps by random) from this set of points. Then the algorithm exchanges points that are in the grid but not in the design with points currently in the design in an effort to improve the selected optimality criterion. Because not every possible design is explicitly evaluated, there is no guarantee that an optimal design has been found, but the exchange procedure usually ensures that a design that is "close" to optimal results. Some implementations repeat the design construction process several times, starting from different initial designs, to increase the likelihood that a final design that is very near the optimal will result.

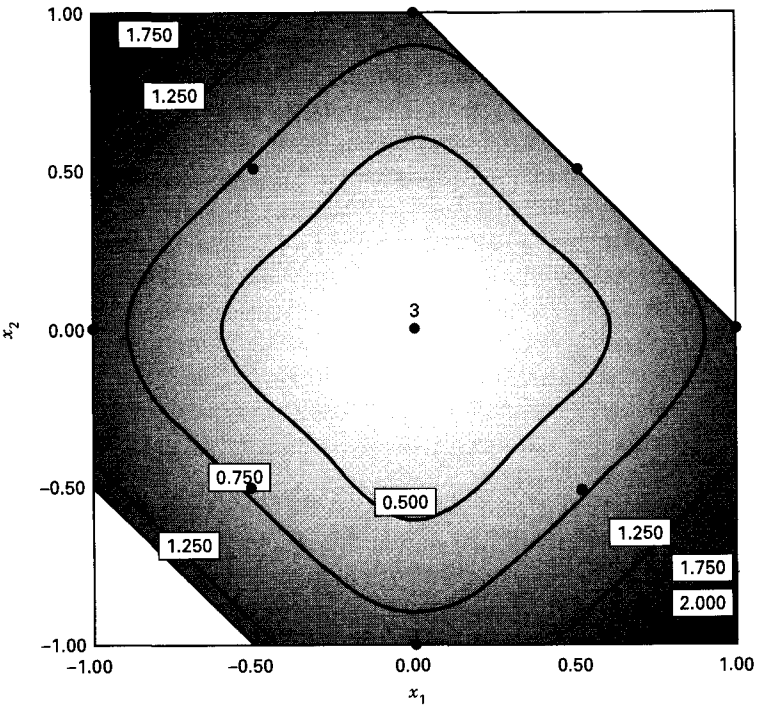
To illustrate some of these ideas, consider the adhesive experiment discussed previously that led to the irregular experimental region in Figure 11-26. Suppose that the response of interest is pull-off force and that we wish to fit a second-order model to this response. In Figure 11-27*a* (page 470) we show a central composite design with four center points (12 runs total) inscribed inside this region. This is not a rotatable design, but it is the largest CCD that we can fit inside the design space. For this design $|(\mathbf{X}'\mathbf{X})^{-1}| = 1.852$ E-2, and the trace of $(\mathbf{X}'\mathbf{X})^{-1}$ is 6.375. Also shown in Figure 11-27*a* are the contours of constant standard deviation of the predicted response, calculated assuming that $\sigma = 1$. Figure 11-27*b* shows the corresponding response surface plot.

Figure 11-28*a* (page 471) and Table 11-12 (page 472) show a 12-run D-optimal design for this problem, generated with the Design-Expert software package. For this design, $|(\mathbf{X}'\mathbf{X})^{-1}| = 2.153$ E-4. Notice that the D-criterion is considerably better for this design than for the inscribed CCD. The relative efficiency of the inscribed CCD to the D-optimal design is

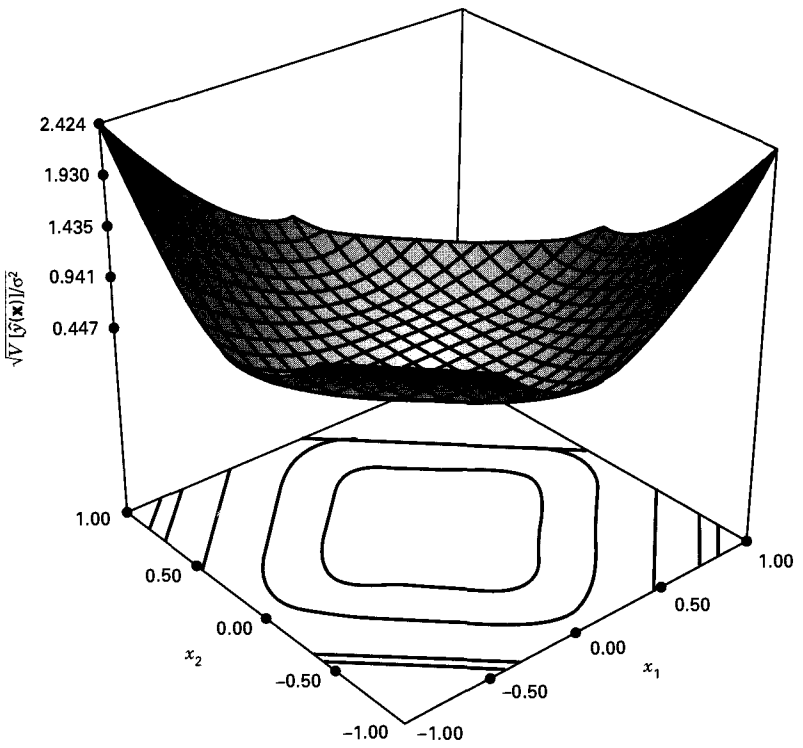
$$D_e = \left(\frac{|(\mathbf{X}_2'\mathbf{X}_2)^{-1}|}{|(\mathbf{X}_1'\mathbf{X}_1)^{-1}|}\right)^{1/p} = \left(\frac{0.0002153}{0.01852}\right)^{1/6} = 0.476$$

That is, the inscribed CCD is only 47.6 percent as efficient as the D-optimal design. This implies that the CCD would have to be replicated 1/0.476 = 2.1 times (or approximately twice) to have the same precision of estimation for the regression coefficients as achieved with the D-optimal design. The trace of $(\mathbf{X}'\mathbf{X})^{-1}$ is 2.516 for the D-optimal design, indicating that the sum of the variances of the regression coefficients are considerably smaller for this design than for the CCD. Figure 11-28*a* and *b* also shows the contours of constant standard deviation of predicted response and the associated response surface plot (assuming that $\sigma = 1$). Generally, the prediction standard deviation contours are lower for the D-optimal design than for the inscribed CCD, particularly near the boundaries of the region of interest where the inscribed CCD does not have any design points.

Figure 11-29*a* (page 473) shows a third design, created by taking the two replicates at the corners of the region in the D-optimal design and moving them to the design center. This could be a useful idea, because Figure 11-28*b* shows that the standard deviation of predicted response increases slightly near the center of the design region for the D-optimal design. Figure 11-29*a* also shows the contours of constant standard de-

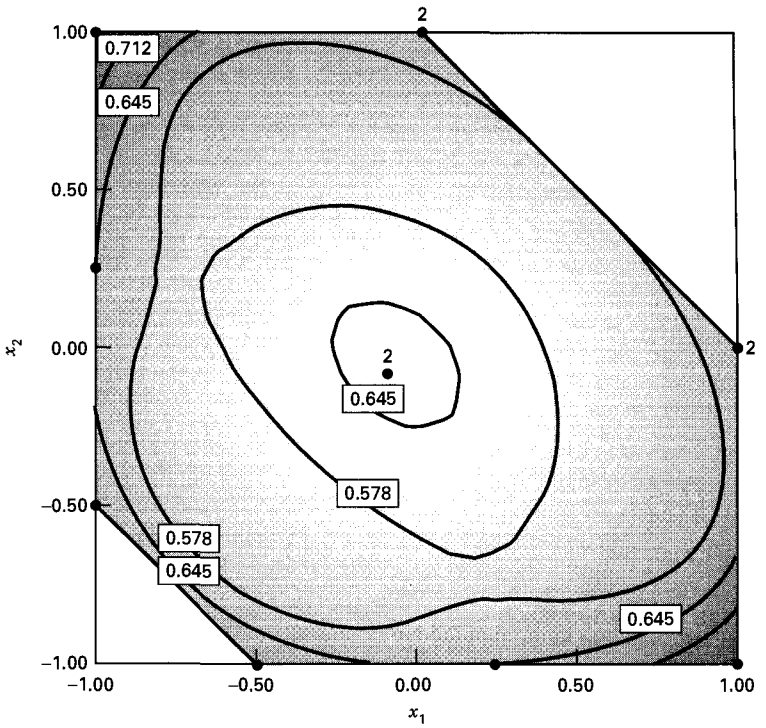


(*a*) The design and contours of constant $\sqrt{V[\hat{y}(\mathbf{x})]/\sigma^2}$

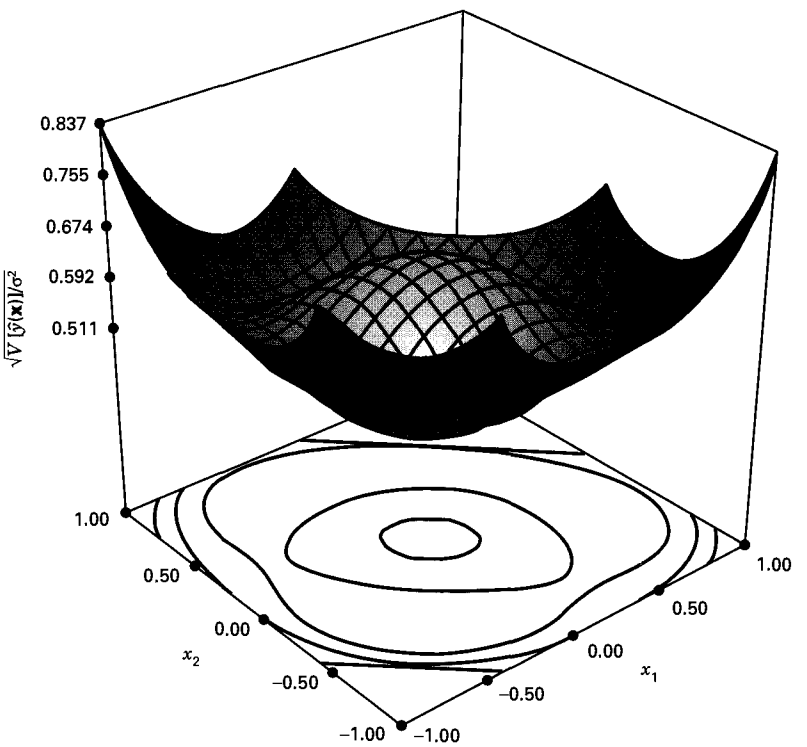


(*b*) The response surface plot

Figure 11-27 An inscribed central composite design for the constrained design region in Figure 11-26.



(*a*) The design and contours of constant $\sqrt{V[\hat{y}(\mathbf{x})]/\sigma^2}$



(*b*) The response surface plot

Figure 11-28 A *D*-optimal design for the constrained design region in Figure 11-26.

Table 11-12 A *D*-Optimal Design for the Constrained Region in Figure 11-26

Standard Order	x_1	x_2
1	−0.50	−1.00
2	1.00	0.00
3	−0.08	−0.08
4	−1.00	1.00
5	1.00	−1.00
6	0.00	1.00
7	−1.00	0.25
8	0.25	−1.00
9	−1.00	−0.50
10	1.00	0.00
11	0.00	1.00
12	−0.08	−0.08

viation of prediction for this *modified* *D*-optimal design, and Figure 11-29*b* shows the response surface plot. The *D*-criterion for this design is $|(\mathbf{X}'\mathbf{X})^{-1}| = 3.71$ E-4, and the relative efficiency is

$$D_e = \left(\frac{|(\mathbf{X}_2'\mathbf{X}_2)^{-1}|}{|(\mathbf{X}_1'\mathbf{X}_1)^{-1}|}\right)^{1/p} = \left(\frac{0.0002153}{0.000371}\right)^{1/6} = 0.91$$

That is, this design is almost as efficient as the *D*-optimal design. The trace of $(\mathbf{X}'\mathbf{X})^{-1}$ is 2.448 for this design, a slightly larger value than was obtained for the *D*-optimal design. The contours of constant prediction standard deviation for this design visually look at least as good as those for the *D*-optimal design, particularly in the center of the region.

Computer-generated designs based on alphabetic optimality criteria can certainly be useful in situations where the experimental region is not either spherical or cuboidal. However, they are not replacements for standard designs in most problems. Alphabetically optimal designs are generated by strict adherence to one criterion only, and as we noted at the start of Section 11-4, where several different design criteria were listed, including several that are somewhat qualitative or subjective in nature. In real experimental problems, there are usually many criteria that need to be evaluated in selecting a design. For more discussion on this issue, refer to Myers and Montgomery (1995, Chapter 8).

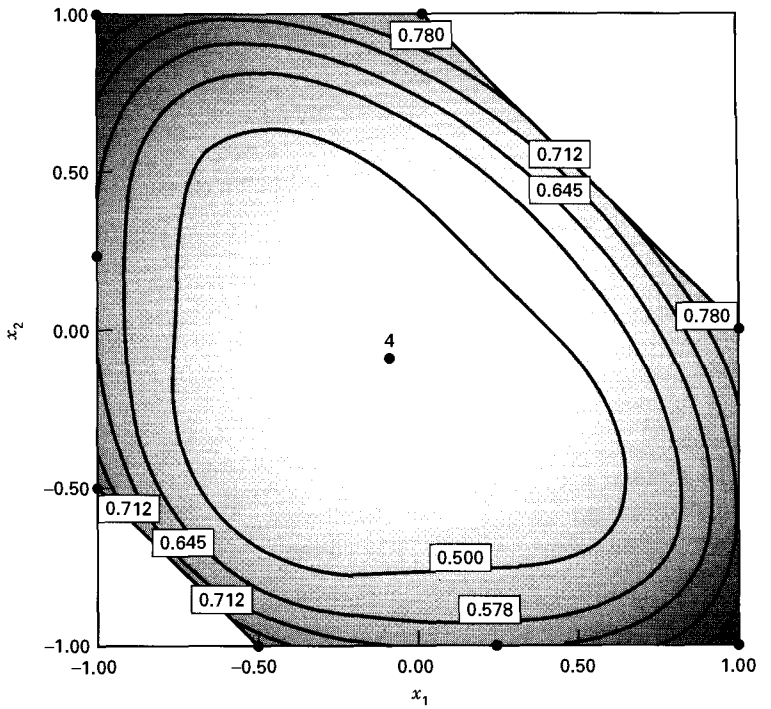
11-5 MIXTURE EXPERIMENTS

In previous sections, we have presented response surface designs for those situations in which the levels of each factor are independent of the levels of other factors. In **mixture experiments**, the factors are the components or ingredients of a mixture, and consequently, their levels are not independent. For example, if $x_1, x_2, \ldots, x_p$ denote the proportions of p components of a mixture, then

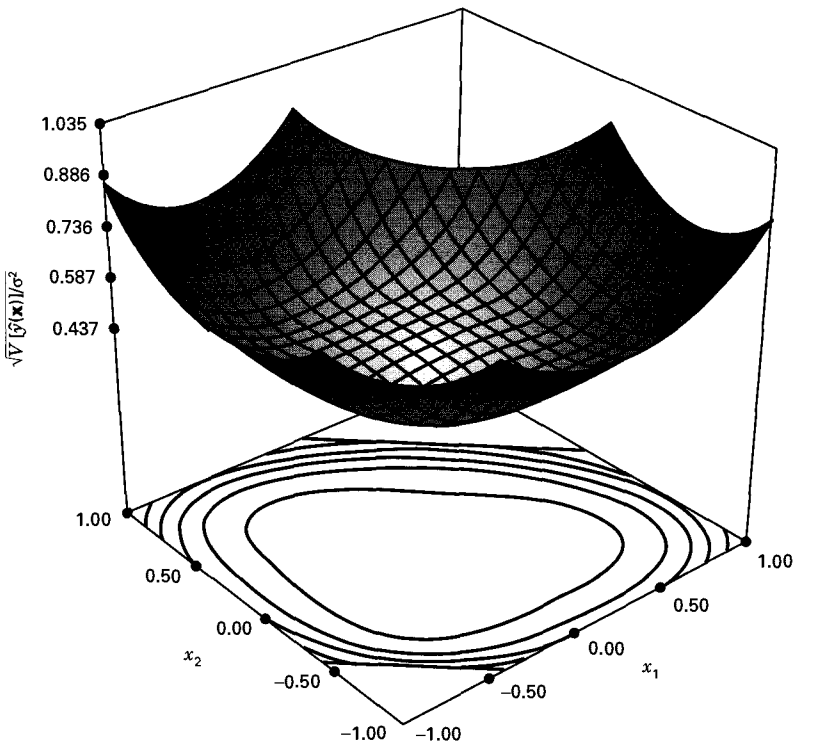
$$0 \leq x_i \leq 1 \qquad i = 1, 2, \ldots, p$$

and

$$x_1 + x_2 + \cdots + x_p = 1 \qquad \text{(i.e., 100 percent)}$$



(*a*) The design and contours of constant $\sqrt{V[\hat{y}(\mathbf{x})]/\sigma^2}$



(*b*) The response surface plot

Figure 11-29 A modified *D*-optimal design for the constrained design region in Figure 11-26.

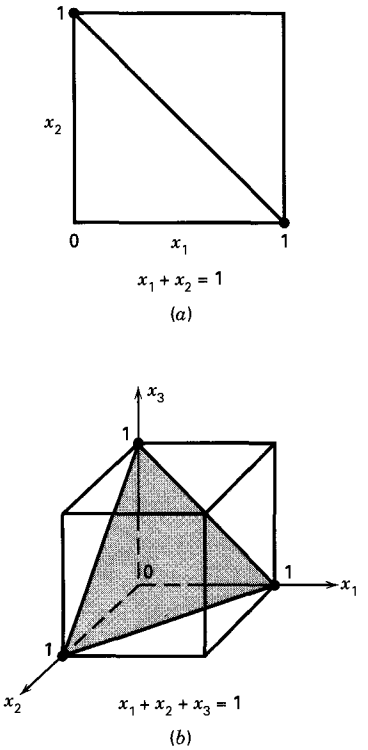


Figure 11-30 Constrained factor space for mixtures with (*a*) $p = 2$ components and (*b*) $p = 3$ components.

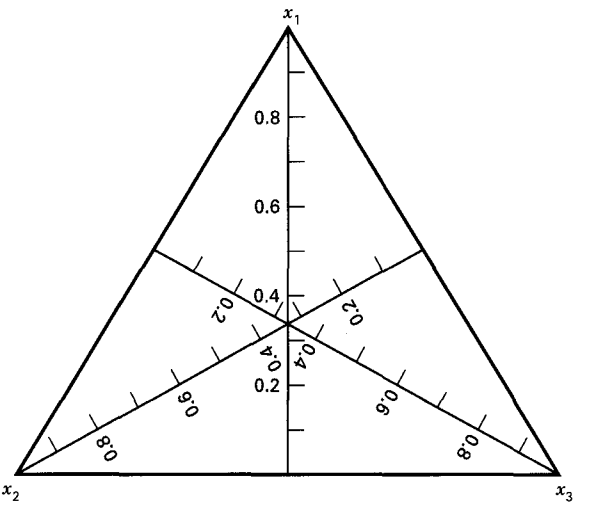


Figure 11-31 Trilinear coordinate system.

These restrictions are illustrated graphically in Figure 11-30 for $p = 2$ and $p = 3$ components. For two components, the factor space for the design includes all values of the two components that lie on the line segment $x_1 + x_2 = 1$, with each component being bounded by 0 and 1. With three components, the mixture space is a triangle with vertices corresponding to formulations that are **pure blends** (mixtures that are 100 percent of a single component).

When there are three components of the mixture, the constrained experimental region can be conveniently represented on **trilinear coordinate paper** as shown in Figure 11-31. Each of the three sides of the graph in Figure 11-31 represents a mixture that has none of one of the three components (the component labeled on the opposite vertex). The nine grid lines in each direction mark off 10 percent increments in the respective components.

Simplex designs are used to study the effects of mixture components on the response variable. A $\{p, m\}$ **simplex lattice design** for p components consists of points defined by the following coordinate settings: the proportions assumed by each component take the $m + 1$ equally spaced values from 0 to 1,

$$x_i = 0, \frac{1}{m}, \frac{2}{m}, \ldots, 1 \qquad i = 1, 2, \ldots, p \tag{11-21}$$

and all possible combinations (mixtures) of the proportions from Equation 11-21 are used. As an example, let $p = 3$ and $m = 2$. Then

$$x_i = 0, \tfrac{1}{2}, 1 \qquad i = 1, 2, 3$$

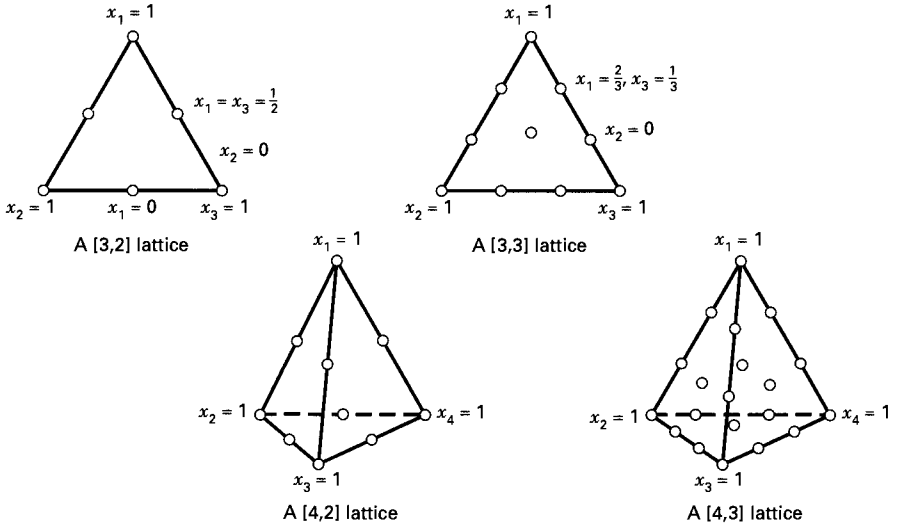


Figure 11-32 Some simplex lattice designs for $p = 3$ and $p = 4$ components.

and the simplex lattice consists of the following six runs:

$$(x_1, x_2, x_3) = (1, 0, 0), (0, 1, 0), (0, 0, 1), (\tfrac{1}{2}, \tfrac{1}{2}, 0), (\tfrac{1}{2}, 0, \tfrac{1}{2}), (0, \tfrac{1}{2}, \tfrac{1}{2})$$

This design is shown in Figure 11-32. The three vertices (1, 0, 0), (0, 1, 0), and (0, 0, 1) are the pure blends, whereas the points $(\frac{1}{2}, \frac{1}{2}, 0)$, $(\frac{1}{2}, 0, \frac{1}{2})$, and $(0, \frac{1}{2}, \frac{1}{2})$ are binary blends or two-component mixtures located at the midpoints of the three sides of the triangle. Figure 11-32 also shows the {3, 3}, {4, 2}, and {4, 3} simplex lattice designs. In general, the number of points in a $\{p, m\}$ simplex lattice design is

$$N = \frac{(p + m - 1)!}{m!(p - 1)!}$$

An alternative to the simplex lattice design is the **simplex centroid design**. In a p-component simplex centroid design, there are $2^p - 1$ points, corresponding to the p permutations of (1, 0, 0, . . . , 0), the $\binom{p}{2}$ permutations of $(\frac{1}{2}, \frac{1}{2}, 0, \ldots, 0)$, the $\binom{p}{3}$ permutations of $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0, \ldots, 0), \ldots$, and the overall centroid $(\frac{1}{p}, \frac{1}{p}, \ldots, \frac{1}{p})$. Figure 11-33 shows some simplex centroid designs.

A criticism of the simplex designs described above is that most of the experimental

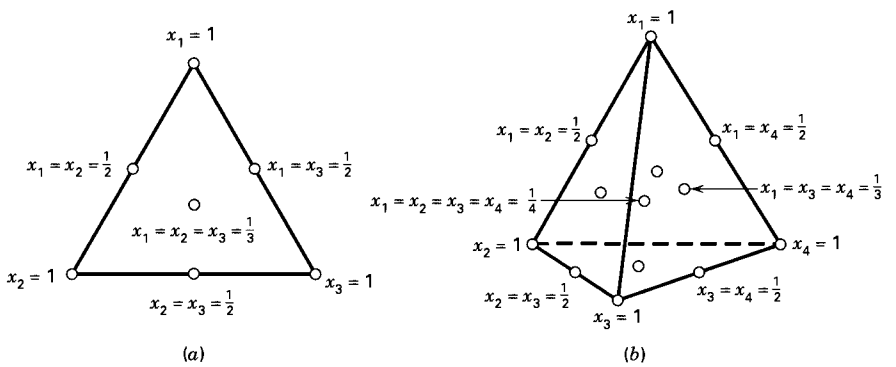

$x_1 = 1$
$x_1 = x_2 = \frac{1}{2}$
$x_1 = x_3 = \frac{1}{2}$
$x_1 = x_2 = x_3 = \frac{1}{3}$
$x_2 = 1$
$x_3 = 1$
$x_2 = x_3 = \frac{1}{2}$
(a)
$x_1 = 1$
$x_1 = x_2 = \frac{1}{2}$
$x_1 = x_4 = \frac{1}{2}$
$x_1 = x_2 = x_3 = x_4 = \frac{1}{4}$
$x_1 = x_3 = x_4 = \frac{1}{3}$
$x_2 = 1$
$x_4 = 1$
$x_2 = x_3 = \frac{1}{2}$
$x_3 = x_4 = \frac{1}{2}$
$x_3 = 1$
(b)

Figure 11-33 Simplex centroid designs with (*a*) $p = 3$ components and (*b*) $p = 4$ components.

runs occur on the boundary of the region and, consequently, include only $p - 1$ of the p components. It is usually desirable to augment the simplex lattice or simplex centroid with additional points in the interior of the region where the blends will consist of all p mixture components. For more discussion, see Cornell (1990) and Myers and Montgomery (1995).

Mixture models differ from the usual polynomials employed in response surface work because of the constraint $\Sigma x_i = 1$. The standard forms of the mixture models that are in widespread use are

Linear:

$$E(y) = \sum_{i=1}^{p} \beta_i x_i \tag{11-22}$$

Quadratic:

$$E(y) = \sum_{i=1}^{p} \beta_i x_i + \sum \sum_{i<j}^{p} \beta_{ij} x_i x_j \tag{11-23}$$

Full Cubic:

$$\begin{aligned} E(y) = &\sum_{i=1}^{p} \beta_i x_i + \sum \sum_{i<j}^{p} \beta_{ij} x_i x_j \\ &+ \sum \sum_{i<j}^{p} \delta_{ij} x_i x_j (x_i - x_j) \\ &+ \sum \sum \sum_{i<j<k} \beta_{ijk} x_i x_j x_k \end{aligned} \tag{11-24}$$

Special Cubic:

$$\begin{aligned} E(y) = &\sum_{i=1}^{p} \beta_i x_i + \sum \sum_{i<j}^{p} \beta_{ij} x_i x_j \\ &+ \sum \sum \sum_{i<j<k} \beta_{ijk} x_i x_j x_k \end{aligned} \tag{11-25}$$

The terms in these models have relatively simple interpretations. In Equations 11-22 through 11-25, the parameter β_i represents the expected response to the pure blend $x_i = 1$ and $x_j = 0$ when $j \neq i$. The portion $\Sigma_{i=1}^{p} \beta_i x_i$ is called the **linear blending portion.** When there is curvature arising from nonlinear blending between component pairs, the parameters β_{ij} represent either **synergistic** or **antagonistic blending.** Higher-order terms are frequently necessary in mixture models because (1) the phenomena studied may be complex and (2) the experimental region is frequently the entire operability region and is therefore large, requiring an elaborate model.

EXAMPLE 11-3

A Three-Component Mixture

Cornell (1990) describes a mixture experiment in which three components—polyethylene (x_1), polystyrene (x_2), and polypropylene (x_3)—were blended to form fiber that will be spun into yarn for draperies. The response variable of interest is yarn elongation in kilograms of force applied. A {3, 2} simplex lattice design is used to study the product. The design and the observed responses are shown in Table 11-13 on the next page. Notice

Table 11-13 The {3, 2} Simplex Lattice Design for the Yarn Elongation Problem

Design Point	Component Proportions x_1	x_2	x_3	Observed Elongation Values	Average Elongation Value ($\bar{y}$)
1	1	0	0	11.0, 12.4	11.7
2	$\frac{1}{2}$	$\frac{1}{2}$	0	15.0, 14.8, 16.1	15.3
3	0	1	0	8.8, 10.0	9.4
4	0	$\frac{1}{2}$	$\frac{1}{2}$	10.0, 9.7, 11.8	10.5
5	0	0	1	16.8, 16.0	16.4
6	$\frac{1}{2}$	0	$\frac{1}{2}$	17.7, 16.4, 16.6	16.9

that all of the design points involve either **pure** or **binary blends**; that is, at most only two of the three components are used in any formulation of the product. Replicate observations are also run, with two replicates at each of the pure blends and three replicates at each of the binary blends. The error standard deviation can be estimated from these replicate observations as $\hat{\sigma} = 0.85$. Cornell fits the second-order mixture polynomial to the data, resulting in

$$\hat{y} = 11.7x_1 + 9.4x_2 + 16.4x_3 + 19.0x_1x_2 + 11.4x_1x_3 - 9.6x_2x_3$$

This model can be shown to be an adequate representation of the response. Note that because $\hat{\beta}_3 > \hat{\beta}_1 > \hat{\beta}_2$, we would conclude that component 3 (polypropylene) produces yarn with the highest elongation. Furthermore, because $\hat{\beta}_{12}$ and $\hat{\beta}_{13}$ are positive, blending components 1 and 2 or components 1 and 3 produces higher elongation values than would be expected just by averaging the elongations of the pure blends. This is an example of "synergistic" blending effects. Components 2 and 3 have antagonistic blending effects because $\hat{\beta}_{23}$ is negative.

Figure 11-34 plots the contours of elongation, and this may be helpful in interpreting the results. From examining the figure, we note that if maximum elongation is desired, a blend of components 1 and 3 should be chosen consisting of about 80 percent component 3 and 20 percent component 1.

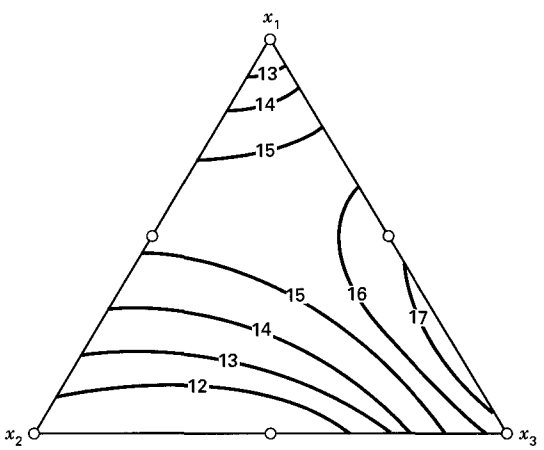


Figure 11-34 Contours of constant estimated yarn elongation from the second-order mixture model for Example 11-3.

We noted previously that the simplex lattice and simplex centroid designs are **boundary point designs**. If the experimenter wants to make predictions about the properties of complete mixtures, it would be highly desirable to have more runs in the interior of the simplex. We recommend augmenting the usual simplex designs with **axial runs** and the overall centroid (if the centroid is not already a design point).

The **axis of component** i is the line or ray extending from the base point $x_i = 0$, $x_j = 1/(p-1)$ for all $j \neq i$ to the opposite vertex where $x_i = 1$, $x_j = 0$ for all $j \neq i$. The base point will always lie at the centroid of the $(p-2)$-dimensional boundary of the simplex that is opposite the vertex $x_i = 1, x_j = 0$ for all $j \neq i$. [The boundary is sometimes called a $(p-2)$-flat.] The length of the component axis is one unit. **Axial points** are positioned along the component axes a distance Δ from the centroid. The maximum value for Δ is $(p-1)/p$. We recommend that axial runs be placed midway between the centroid of the simplex and each vertex so that $\Delta = (p-1)/2p$. Sometimes these points are called **axial check blends** because a fairly common practice is to exclude them when fitting the preliminary mixture model and then use the responses at these axial points to check the adequacy of the fit of the preliminary model.

Figure 11-35 shows the $\{3, 2\}$ simplex lattice design augmented with the axial points. This design has 10 points, with four of these points in the interior of the simplex. The $\{3, 3\}$ simplex lattice will support fitting the full cubic model, whereas the augmented simplex lattice will not; however, the augmented simplex lattice will allow the experimenter to fit the special cubic model or to add special quartic terms such as $\beta_{1233}x_1x_2x_3^2$ to the quadratic model. The augmented simplex lattice is superior for studying the response of complete mixtures in the sense that it can detect and model curvature in the interior of the triangle that cannot be accounted for by the terms in the full cubic model. The augmented simplex lattice has more power for detecting lack of fit than does the $\{3, 3\}$ lattice. This is particularly useful when the experimenter is unsure about the proper model to use and also plans to sequentially build a model by starting with a simple

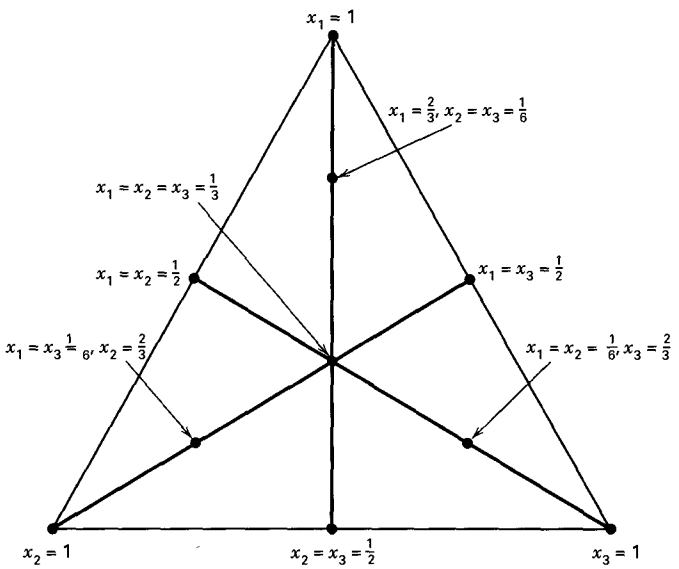

$x_1 = 1$
$x_1 = \frac{2}{3}, x_2 = x_3 = \frac{1}{6}$
$x_1 = x_2 = x_3 = \frac{1}{3}$
$x_1 = x_2 = \frac{1}{2}$
$x_1 = x_3 = \frac{1}{2}$
$x_1 = x_3 = \frac{1}{6}, x_2 = \frac{2}{3}$
$x_1 = x_2 = \frac{1}{6}, x_3 = \frac{2}{3}$
$x_2 = 1$
$x_2 = x_3 = \frac{1}{2}$
$x_3 = 1$

Figure 11-35 An augmented simplex-lattice design.

polynomial (perhaps first order), test the model for lack of fit, then augment the model with higher-order terms, test the new model for lack of fit, and so forth.

In some mixture problems, **constraints** on the individual components arise. Lower bound constraints of the form

$$l_i \leq x_i \leq 1 \qquad i = 1, 2, \ldots, p$$

are fairly common. When only lower bound constraints are present, the feasible design region is still a simplex, but it is inscribed inside the original simplex region. This situation may be simplified by the introduction of **pseudocomponents**, defined as

$$x_i' = \frac{x_i - l_i}{\left(1 - \sum_{j=1}^{p} l_j\right)} \tag{11-26}$$

with $\Sigma_{j=1}^{p} l_j < 1$. Now

$$x_1' + x_2' + \cdots + x_p' = 1$$

so the use of pseudocomponents allows the use of simplex-type designs when lower bounds are a part of the experimental situation. The formulations specified by the simplex design for the pseudocomponents are transformed into formulations for the original components by reversing the transformation Equation 11-26. That is, if x_i' is the value assigned to the ith pseudocomponent on one of the runs in the experiment, the ith original mixture component is

$$x_i = l_i + \left(1 - \sum_{j=1}^{p} l_j\right) x_i' \tag{11-27}$$

If the components have both upper and lower bound constraints, the feasible region is no longer a simplex; instead, it will be an irregular polytope. Because the experimental region is not a "standard" shape, **computer-generated designs** are very useful for these types of mixture problems.

EXAMPLE 11-4

Paint Formulation

An experimenter is trying to optimize the formulation of automotive clear coat paint. These are complex products that have very specific performance requirements. Specifically, the customer wants the Knoop hardness to exceed 25 and the percentage of solids to be below 30. The clear coat is a three component mixture, consisting of a monomer (x_1), a crosslinker (x_2), and a resin (x_3). There are constraints on the component proportions:

$$\begin{aligned} x_1 + x_2 + x_3 &= 100 \\ 5 \leq x_1 &\leq 25 \\ 25 \leq x_2 &\leq 40 \\ 50 \leq x_3 &\leq 70 \end{aligned}$$

The result is the constrained region of experimentation shown in Figure 11-36 on the next page. Because the region of interest is not a simplex, we will use a D-optimal design for this problem. Assuming that both responses are likely to be modeled with a quadratic

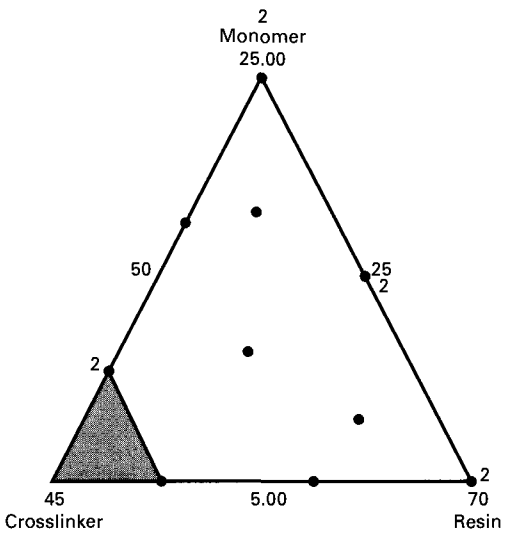


Figure 11-36 The constrained experimental region for the paint formulation problem in Example 11-4 (shown in the actual component scale).

Table 11-14 A *D*-Optimal Design for the Paint Formulation Problem in Example 11-4

Standard Order	Run	Monomer x_1	Crosslinker x_2	Resin x_3	Hardness y_1	Solids y_2
1	2	17.50	32.50	50.00	29	9.539
2	1	10.00	40.00	50.00	26	27.33
3	4	15.00	25.00	60.00	17	29.21
4	13	25.00	25.00	50.00	28	30.46
5	7	5.00	25.00	70.00	35	74.98
6	3	5.00	32.50	62.50	31	31.5
7	6	11.25	32.50	56.25	21	15.59
8	11	5.00	40.00	55.00	20	19.2
9	10	18.13	28.75	53.13	29	23.44
10	14	8.13	28.75	63.13	25	32.49
11	12	25.00	25.00	50.00	19	23.01
12	9	15.00	25.00	60.00	14	41.46
13	5	10.00	40.00	50.00	30	32.98
14	8	5.00	25.00	70.00	23	70.95

Table 11-15 Model Fitting for the Hardness Response

Response: hardness
ANOVA for Mixture Quadratic Model
Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	279.73	5	55.95	2.37	0.1329
Linear Mixture	*29.13*	*2*	*14.56*	*0.62*	*0.5630*
AB	*72.61*	*1*	*72.61*	*3.08*	*0.1174*
AC	*179.67*	*1*	*179.67*	*7.62*	*0.0247*
BC	*8.26*	*1*	*8.26*	*0.35*	*0.5703*
Residual	188.63	8	23.58		
Lack of Fit	*63.63*	*4*	*15.91*	*0.51*	*0.7354*
Pure Error	*125.00*	*4*	*31.25*		
Cor Total	468.36	13			

Std. Dev.	4.86	R-Squared	0.5973
Mean	24.79	Adj R-Squared	0.3455
C.V.	19.59	Pred R-Squared	−0.3635
PRESS	638.60	Adeq Precision	4.975

Component	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High
A-Monomer	23.81	1	3.36	16.07	31.55
B-Crosslinker	16.40	1	7.68	−1.32	34.12
C-Resin	29.45	1	3.36	21.71	37.19
AB	44.42	1	25.31	−13.95	102.80
AC	−44.01	1	15.94	−80.78	−7.25
BC	13.80	1	23.32	−39.97	67.57

Final Equation in Terms of Pseudo Components:

hardness =
+23.81 * A
+16.40 * B
+29.45 * C
+44.42 * A * B
−44.01 * A * C
+13.80 * B * C

mixture model, we can generate the *D*-optimal design shown in Figure 11-36 using Design-Expert. We assumed that in addition to the six runs required to fit the quadratic mixture model that four additional distinct runs would be made to check for lack of fit and that four of these runs would be replicated to provide an estimate of pure error. Design-Expert used the vertices, the edge centers, the overall centroid and the check runs (points located halfway between the centroid and the vertices) as the candidate points.

The 14-run design is shown in Table 11-14 (page 480), along with the hardness and solids responses. The results of fitting quadratic models to both responses are summarized in Tables 11-15 and 11-16 (pages 481 and 482). Notice that quadratic models fit nicely to both the hardness and the solids responses. The fitted equations for both responses (in terms of the pseudocomponents) are shown in these tables. Contour plots of the responses are shown in Figures 11-37 and 11-38 (pages 482 and 483).

Figure 11-39 (page 483) is an overlay plot of the two response surfaces, showing the Knoop hardness contour of 25 and the 30 percent contour for solids. The feasible region for this product is the unshaded region near the center of the plot. Obviously,

Table 11-16 Model Fitting for the Solids Response

Response: solids
ANOVA for Mixture Quadratic Model
Analysis of variance table [Partial sum of squares]

Source	Sum of Squares	DF	Mean Square	F Value	Prob > F
Model	4297.94	5	859.59	25.78	<0.0001
Linear Mixture	*2931.09*	*2*	*1465.66*	*43.95*	*<0.0001*
AB	*211.20*	*1*	*211.20*	*6.33*	*0.0360*
AC	*285.67*	*1*	*285.67*	*8.57*	*0.0191*
BC	*1036.72*	*1*	*1036.72*	*31.09*	*0.0005*
Residual	266.79	8	33.35		
Lack of Fit	*139.92*	*4*	*34.98*	*1.10*	*0.4633*
Pure Error	*126.86*	*4*	*31.72*		
Cor Total	4564.73	13			

Std. Dev.	5.77	R-Squared	0.9416
Mean	33.01	Adj R-Squared	0.9050
C.V.	17.49	Pred R-Squared	0.7827
PRESS	991.86	Adeq Precision	15.075

Component	Coefficient Estimate	DF	Standard Error	95%CI Low	95% CI High
A-Monomer	26.53	1	3.99	17.32	35.74
B-Crosslinker	46.60	1	9.14	25.53	67.68
C-Resin	73.23	1	3.99	64.02	82.43
AB	−75.76	1	30.11	−145.19	−6.34
AC	−55.50	1	18.96	−99.22	−11.77
BC	−154.61	1	27.73	−218.56	−90.67

Final Equation in Terms of Pseudo Components:

solids =
+26.53 * A
+46.60 * B
+73.23 * C
−75.76 * A * B
−55.50 * A * C
−154.61 * B * C

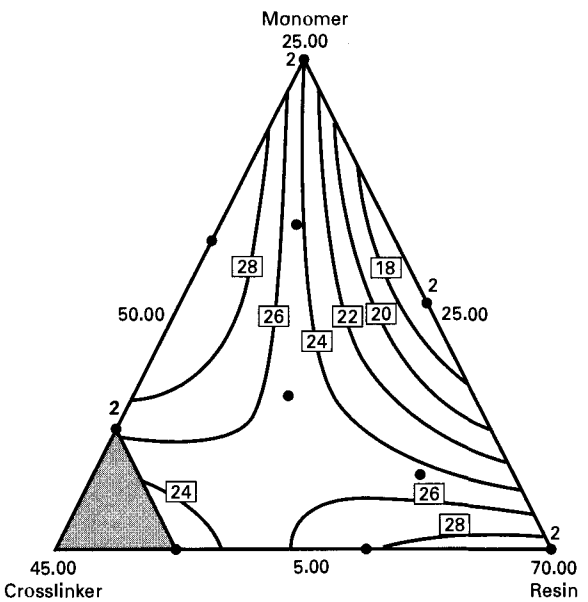


Figure 11-37 Contour plot of the Knoop hardness response, Example 11-4.

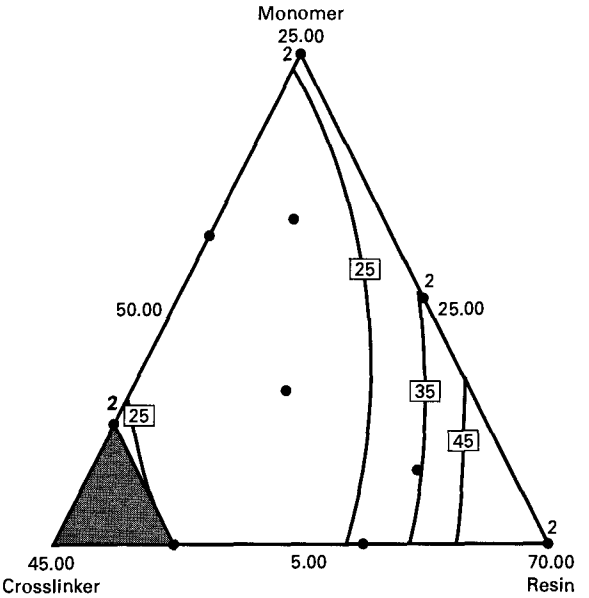


Figure 11-38 Contour plot of the percentage of solids response, Example 11-4.

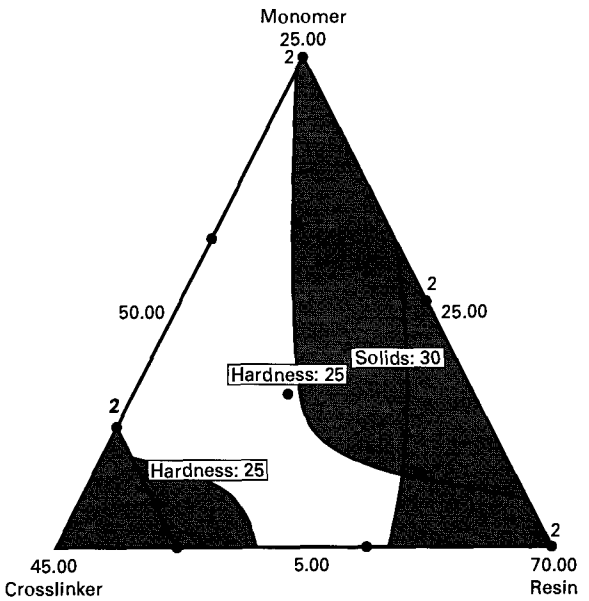


Figure 11-39 Overlay plot of the Knoop hardness and percentage of solids response, showing the feasible region for the paint formulation.

there are a number of choices for the proportions of monomer, crosslinker, and resin for the clear coat that will give a product satisfying the performance requirements.

11-6 EVOLUTIONARY OPERATION

Response surface methodology is often applied to pilot plant operations by research and development personnel. When it is applied to a full-scale production process, it is usually only done once (or very infrequently) because the experimental procedure is relatively elaborate. However, conditions that were optimum for the pilot plant may not be optimum for the full-scale process. The pilot plant may produce 2 pounds of product per day, whereas the full-scale process may produce 2000 pounds per day. This "scale-up" of the pilot plant to the full-scale production process usually results in distortion of the optimum conditions. Even if the full-scale plant begins operation at the optimum, it will eventually "drift" away from that point because of variations in raw materials, environmental changes, and operating personnel.

A method is needed for the continuous monitoring and improvement of a full-scale process with the goal of moving the operating conditions toward the optimum or following a "drift." The method should not require large or sudden changes in operating conditions that might disrupt production. **Evolutionary operation (EVOP)** was proposed by Box (1957) as such an operating procedure. It is designed as a method of routine plant operation that is carried out by manufacturing personnel with minimum assistance from the research and development staff.

EVOP consists of systematically introducing small changes in the levels of the operating variables under consideration. Usually, a 2^k design is employed to do this. The changes in the variables are assumed to be small enough that serious disturbances in yield, quality, or quantity will not occur, yet large enough that potential improvements in process performance will eventually be discovered. Data are collected on the response variables of interest at each point of the 2^k design. When one observation has been taken at each design point, a **cycle** is said to have been completed. The effects and interactions of the process variables may then be computed. Eventually, after several cycles, the effect of one or more process variables or their interactions may appear to have a significant effect on the response. At this point, a decision may be made to change the basic operating conditions to improve the response. When improved conditions have been detected, a **phase** is said to have been completed.

In testing the significance of process variables and interactions, an estimate of experimental error is required. This is calculated from the cycle data. Also, the 2^k design is usually centered about the current best operating conditions. By comparing the response at this point with the 2^k points in the factorial portion, we may check on curvature or **change in mean** (CIM); that is, if the process is really centered at the maximum, say, then the response at the center should be significantly greater than the responses at the 2^k-peripheral points.

In theory, EVOP can be applied to k process variables. In practice, only two or three variables are usually considered. We will give an example of the procedure for two variables. Box and Draper (1969) give a detailed discussion of the three-variable case, including necessary forms and worksheets. Myers and Montgomery (1995) discuss the computer implementation of EVOP.

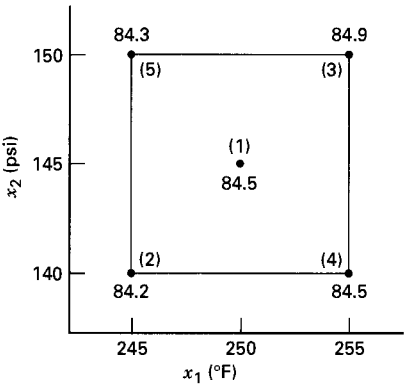


Figure 11-40 A 2^2 design for EVOP.

EXAMPLE 11-5

Consider a chemical process whose yield is a function of temperature (x_1) and pressure (x_2). The current operating conditions are $x_1 = 250$°F and $x_2 = 145$ psi. The EVOP procedure uses the 2^2 design plus the center point shown in Figure 11-40. The cycle is completed by running each design point in numerical order (1, 2, 3, 4, 5). The yields in the first cycle are also shown in Figure 11-40.

The yields from the first cycle are entered in the EVOP calculation sheet, shown in Table 11-17. At the end of the first cycle, no estimate of the standard deviation can be

Table 11-17 EVOP Calculation Sheet for Example 11-5, $n = 1$

5 3 / 2 •1 4	Cycle: $n = 1$ Response: Yield					Phase: 1 Date: 1/11/00
	Calculation of Averages					Calculation of Standard Deviation
Operating Conditions	(1)	(2)	(3)	(4)	(5)	
(i) Previous cycle sum						Previous sum S =
(ii) Previous cycle average						Previous average S =
(iii) New observations	84.5	84.2	84.9	84.5	84.3	New S = range × $f_{5,n}$ =
(iv) Differences [(ii) − (iii)]						Range of (iv) =
(v) New sums [(i) + (iii)]	84.5	84.2	84.9	84.5	84.3	New sum S =
(vi) New averages [$\bar{y}_i$ = (v)/n]	84.5	84.2	84.9	84.5	84.3	New average S = $\frac{\text{New sum } S}{n-1}$

Calculation of Effects	Calculation of Error Limits
Temperature effect = $\frac{1}{2}(\bar{y}_3 + \bar{y}_4 - \bar{y}_2 - \bar{y}_5) = 0.45$	For new average = $\frac{2}{\sqrt{n}} S$ =
Pressure effect = $\frac{1}{2}(\bar{y}_3 + \bar{y}_5 - \bar{y}_2 - \bar{y}_4) = 0.25$	For new effects $\frac{2}{\sqrt{n}} S$ =
$T \times P$ interaction effect = $\frac{1}{2}(\bar{y}_2 + \bar{y}_3 - \bar{y}_4 - \bar{y}_5) = 0.15$	
Change-in-mean effect = $\frac{1}{5}(\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5 - 4\bar{y}_1) = 0.02$	For change in mean $\frac{1.78}{\sqrt{n}} S$ =

Table 11-18 EVOP Calculation Sheet for Example 11-5, $n = 2$

Cycle: $n = 2$
Response: Yield

Phase: 1
Date: 1/11/00

Operating Conditions	Calculation of Averages (1)	(2)	(3)	(4)	(5)	Calculation of Standard Deviation
(i) Previous cycle sum	84.5	84.2	84.9	84.5	84.3	Previous sum S =
(ii) Previous cycle average	84.5	84.2	84.9	84.5	84.3	Previous average S =
(iii) New observations	84.9	84.6	85.9	83.5	84.0	New S = range × $f_{5,n} = 0.60$
(iv) Differences [(ii) − (iii)]	−0.4	−0.4	−1.0	+1.0	0.3	Range of (iv) = 2.0
(v) New sums [(i) + (iii)]	169.4	168.8	170.8	168.0	168.3	New sum $S = 0.60$
(vi) New averages [$\bar{y}_i$ = (v)/n]	84.70	84.40	85.40	84.00	84.15	New average $S = \dfrac{\text{New sum } S}{n-1} = 0.60$

Calculation of Effects	Calculation of Error Limits
Temperature effect = $\frac{1}{2}(\bar{y}_3 + \bar{y}_4 - \bar{y}_2 - \bar{y}_5) = 0.43$	For new average = $\dfrac{2}{\sqrt{n}} S = 0.85$
Pressure effect = $\frac{1}{2}(\bar{y}_3 + \bar{y}_5 - \bar{y}_2 - \bar{y}_4) = 0.58$	For new effects $\dfrac{2}{\sqrt{n}} S = 0.85$
$T \times P$ interaction effect = $\frac{1}{2}(\bar{y}_2 + \bar{y}_3 - \bar{y}_4 - \bar{y}_5) = 0.83$	
Change-in-mean effect = $\frac{1}{5}(\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5 - 4\bar{y}_1) = -0.17$	For change in mean $\dfrac{1.78}{\sqrt{n}} S = 0.76$

made. The effects and interaction for temperature and pressure are calculated in the usual manner for a 2^2 design.

A second cycle is then run and the yield data entered in another EVOP calculation sheet, shown in Table 11-18. At the end of the second cycle, the experimental error can be estimated and the estimates of the effects compared to approximate 95 percent (two standard deviation) limits. Note that the range refers to the range of the differences in row (iv); thus the range is $+1.0 - (-1.0) = 2.0$. Because none of the effects in Table 11-18 exceed their error limits, the true effect is probably zero, and no changes in operating conditions are contemplated.

The results of a third cycle are shown in Table 11-19 on the facing page. The effect of pressure now exceeds its error limit and the temperature effect is equal to the error limit. A change in operating conditions is now probably justified.

In light of the results, it seems reasonable to begin a new EVOP phase about point (3). Thus, $x_1 = 225°\text{F}$ and $x_2 = 150$ psi would become the center of the 2^2 design in the second phase.

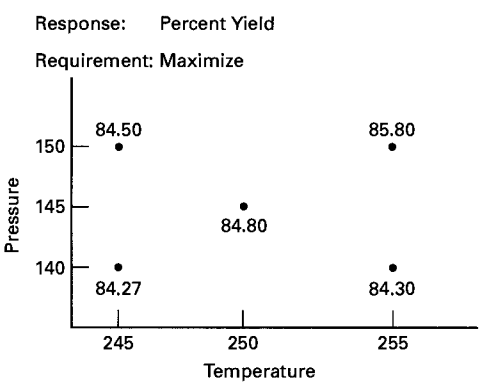
An important aspect of EVOP is feeding the information generated back to the process operators and supervisors. This is accomplished by a prominently displayed EVOP information board. The information board for this example at the end of cycle 3 is shown in Table 11-20 on the facing page.

Table 11-19 EVOP Calculation Sheet for Example 11-5, $n = 3$

5 • 3 / • 1 / 2 • 4	Cycle: $n = 3$ Response: Yield				Phase: 1 Date: 1/11/00
	Calculation of Averages				Calculation of Standard Deviation
Operating Conditions	(1)	(2)	(3)	(4)	(5)	
(i) Previous cycle sum	169.4	168.8	170.8	168.0	168.3	Previous sum $S = 0.60$
(ii) Previous cycle average	84.70	84.40	85.40	84.00	84.15	Previous average $S = 0.60$
(iii) New observations	85.0	84.0	86.6	84.9	85.2	New S = range $\times$ $f_{5,n} = 0.56$
(iv) Differences [(ii) − (iii)]	−0.30	+0.40	−1.20	−0.90	−1.05	Range of (iv) = 1.60
(v) New sums [(i) + (iii)]	254.4	252.8	257.4	252.9	253.5	New sum $S = 1.16$
(vi) New averages [$\bar{y}_i$ = (v)/n]	84.80	84.27	85.80	84.30	84.50	New average $S = \dfrac{\text{New sum } S}{n-1} = 0.58$

Calculation of Effects	Calculation of Error Limits
Temperature effect $= \frac{1}{2}(\bar{y}_3 + \bar{y}_4 - \bar{y}_2 - \bar{y}_5) = 0.67$	For new average $= \dfrac{2}{\sqrt{n}} S = 0.67$
Pressure effect $= \frac{1}{2}(\bar{y}_3 + \bar{y}_5 - \bar{y}_2 - \bar{y}_4) = 0.87$	
$T \times P$ interaction effect $= \frac{1}{2}(\bar{y}_2 + \bar{y}_3 - \bar{y}_4 - \bar{y}_5) = 0.64$	For new effects $\dfrac{2}{\sqrt{n}} S = 0.67$
Change-in-mean effect $= \frac{1}{5}(\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5 - 4\bar{y}_1) = -0.07$	For change in mean $\dfrac{1.78}{\sqrt{n}} S = 0.60$

Table 11-20 EVOP Information Board, Cycle 3



Error Limits for Averages: ±0.67			
Effects with 95 percent error Limits:	Temperature	0.67	±0.67
	Pressure	0.87	±0.67
	$T \times P$	0.64	±0.67
	Change in mean	0.07	±0.60
Standard deviation:	0.58		

Table 11-21 Values of $f_{k,n}$

$n =$	2	3	4	5	6	7	8	9	10
$k = 5$	0.30	0.35	0.37	0.38	0.39	0.40	0.40	0.40	0.41
9	0.24	0.27	0.29	0.30	0.31	0.31	0.31	0.32	0.32
10	0.23	0.26	0.28	0.29	0.30	0.30	0.30	0.31	0.31

Most of the quantities on the EVOP calculation sheet follow directly from the analysis of the 2^k factorial design. For example, the variance of any effect, such as $\frac{1}{2}(\bar{y}_3 + \bar{y}_5 - \bar{y}_2 - \bar{y}_4)$, is simply σ^2/n where σ^2 is the variance of the observations (y). Thus, two standard deviation (corresponding to 95 percent) error limits on any effect would be $\pm 2\sigma/\sqrt{n}$. The variance of the change in mean is

$$V(\text{CIM}) = V\left[\frac{1}{5}(\bar{y}_2 + \bar{y}_3 + \bar{y}_4 + \bar{y}_5 - 4\bar{y}_1)\right]$$
$$= \frac{1}{25}(5\sigma_{\bar{y}}^2 + 16\sigma_{\bar{y}}^2) = \left(\frac{20}{25}\right)\frac{\sigma^2}{n}$$

Thus, two standard deviation error limits on the CIM are $\pm(2\sqrt{20/25})\sigma/\sqrt{n} = \pm 1.78\sigma/\sqrt{n}$.

The standard deviation σ is estimated by the range method. Let $y_i(n)$ denote the observation at the ith design point in cycle n and $\bar{y}_i(n)$ denote the corresponding average of $y_i(n)$ after n cycles. The quantities in row (iv) of the EVOP calculation sheet are the differences $y_i(n) - \bar{y}_i(n-1)$. The variance of these differences is

$$V[y_i(n) - \bar{y}_i(n-1)] \equiv \sigma_D^2 = \sigma^2\left[1 + \frac{1}{(n-1)}\right] = \sigma^2\frac{n}{(n-1)}$$

The range of the differences, say R_D, is related to the estimate of the standard deviation of the differences by $\hat{\sigma}_D = R_D/d_2$. The factor d_2 depends on the number of observations used in computing R_D. Now $R_D/d_2 = \hat{\sigma}\sqrt{n/(n-1)}$, so

$$\hat{\sigma} = \sqrt{\frac{(n-1)}{n}}\frac{R_D}{d_2} = (f_{k,n})R_D \equiv S$$

can be used to estimate the standard deviation of the observations, where k denotes the number of points used in the design. For a 2^2 design with one center point we have $k = 5$, and for a 2^3 design with one center point we have $k = 9$. Values of $f_{k,n}$ are given in Table 11-21.

11-7 ROBUST DESIGN

11-7.1 Background

Throughout this book, we have stressed the importance of using statistically designed experiments for product and process design, development, and improvement. Since about 1980, engineers and scientists have become increasingly aware of the benefits of using designed experiments, and as a consequence, there have been many new application

areas. One of the most important of these is in **robust design**, where the focus is on one or more of the following:

1. Designing systems (products or processes) that are insensitive to environmental factors that can affect performance once the system is deployed in the field. An example is the formulation of an exterior paint that should exhibit long life when exposed to a variety of weather conditions. Because weather conditions are not entirely predictable, and are certainly not constant, the product formulator wants the product to be robust against a wide range of temperature, humidity, and precipitation factors that affect the wear and finish of the paint.
2. Designing products so that they are insensitive to variability transmitted by the components of the system. An example is designing an electronic amplifier so that the output voltage is as close as possible to the desired target regardless of the variability in the electrical parameters of the resistors, transistors, and power supplies that are the components of the device.
3. Designing processes so that the manufactured product will be as close as possible to the desired target specifications even though some process variables (such as temperature) or raw material characteristics are impossible to control precisely.
4. Determining the operating conditions for a process so that critical product characteristics are as close as possible to the desired target value and the variability around this target is minimized. Examples of this type of problem occur frequently. For instance in semiconductor manufacturing we would like the oxide thickness on a wafer to be as close as possible to the target mean thickness, and we would also like for the variability in thickness across the wafer (a measure of uniformity) to be as small as possible.

In the early 1980s, a Japanese engineer, Dr. Genichi Taguchi, introduced an approach to solving these types of problems, which he collectively referred to as the **robust parameter design (RPD)** problem [see Taguchi and Wu (1980), Taguchi (1987, 1991)]. His approach was based on classifying the variables in a process or product as either **control (or controllable) variables** or **noise (or uncontrollable) variables** and then finding the settings for the controllable variables that minimized the variability transmitted to the response from the uncontrollable variables. We make the assumption that although the noise factors are uncontrollable in the full-scale system, they can be controlled for purposes of an experiment. Refer to Figure 1-1 for a graphical view of controllable and uncontrollable variables in the general context of a designed experiment.

Taguchi introduced some novel statistical methods and some variations on established techniques as part of his RPD procedure. He made use of highly fractionated factorial designs and other types of fractional designs obtained from orthogonal arrays. His methodology generated considerable debate and controversy. Part of the controversy arose because Taguchi's methodology was advocated in the West initially (and primarily) by entrepreneurs, and the underlying statistical science had not been adequately peer-reviewed. By the late 1980s the results of a very comprehensive peer review indicated that although Taguchi's engineering concepts and the overall objective of RPD were well-founded, there were substantial problems with his experimental strategy and methods of data analysis. For specific details of these issues, see Box (1988), Box, Bisgaard, and Fung (1988), Hunter (1985) (1989), Montgomery (1999), Myers and Montgomery (1995), and Pignatiello and Ramberg (1992). Many of these concerns are also summa-

Table 11-22 Parameter Design with Both Inner and Outer Arrays

					(b) Outer Array							
					E	1	1	1	1	2	2	2	2
					F	1	1	2	2	1	1	2	2
					G	1	2	1	2	1	2	1	2
	(a) Inner Array												
Run	*A*	*B*	*C*	*D*									
1	1	1	1	1		15.6	9.5	16.9	19.9	19.6	19.6	20.0	19.1
2	1	2	2	2		15.0	16.2	19.4	19.2	19.7	19.8	24.2	21.9
3	1	3	3	3		16.3	16.7	19.1	15.6	22.6	18.2	23.3	20.4
4	2	1	2	3		18.3	17.4	18.9	18.6	21.0	18.9	23.2	24.7
5	2	2	3	1		19.7	18.6	19.4	25.1	25.6	21.4	27.5	25.3
6	2	3	1	2		16.2	16.3	20.0	19.8	14.7	19.6	22.5	24.7
7	3	1	3	2		16.4	19.1	18.4	23.6	16.8	18.6	24.3	21.6
8	3	2	1	3		14.2	15.6	15.1	16.8	17.8	19.6	23.2	24.2
9	3	3	2	1		16.1	19.9	19.3	17.3	23.1	22.7	22.6	28.6

rized in the extensive panel discussion in the May 1992 issue of *Technometrics* [see Nair et al. (1992)]. The supplemental technical material for this chapter also discusses and illustrates many of the problems underlying Taguchi's technical methods.

Taguchi's methodology for the RPD problem revolves around the use of an orthogonal design for the controllable factors that is "crossed" with a separate orthogonal design for the noise factors. Table 11-22 (page 490) presents an example from Byrne and Taguchi (1987) that involved the development of a method to assemble an elastometric connector to a nylon tube that would deliver the required pull-off force. There are four controllable factors, each at three levels (A = interference, B = connector wall thickness, C = insertion depth, D = percent adhesive), and three noise or uncontrollable factors, each at two levels (E = conditioning time, F = conditioning temperature, G = conditioning relative humidity). Panel (a) of Table 11-22 contains the design for the controllable factors. Notice that the design is a three-level fractional factorial; specifically, it is a 3^{4-2} design. Taguchi calls this the **inner array design**. Panel (b) of Table 11-22 contains a 2^3 design for the noise factors, which Taguchi calls the **outer array design**. Now each run in the inner array is performed for all treatment combinations in the outer array, producing the 72 observations on pull-off force shown in the table. This type of design is called a **crossed array design**.

Taguchi suggested that we summarize the data from a crossed array experiment with two statistics: the average of each observation in the inner array across all runs in the outer array and a summary statistic that attempted to combine information about the mean and variance, called the **signal-to-noise ratio**. These signal-to-noise ratios are purportedly defined so that a maximum value of the ratio minimized variability transmitted from the noise variables. Then an analysis is performed to determine which settings of the controllable factors result in (1) the mean as close as possible to the desired target and (2) a maximum value of the signal-to-noise ratio.

Examination of Table 11-22 reveals a major problem with the Taguchi design strategy; namely, the crossed array approach will lead to a very large experiment. In our example, there are only seven factors, yet the design has 72 runs. Furthermore, the inner array design is a 3^{4-2} resolution III design (see Chapter 9 for discussion of this design), so in spite of the large number of runs, we cannot obtain *any* information about interactions among the controllable variables. Indeed, even information about the main effects is potentially tainted because the main effects are heavily aliased with the two-factor interactions. It also turns out that the Taguchi signal-to-noise ratios are problematic; maximizing the ratio does not necessarily minimize variability. Refer to the supplemental text material for more details.

An important point about the crossed array design is that it *does* provide information about controllable factor $\times$ noise factor interactions. These interactions are crucial to the solution of a RPD problem. For example, consider the two-factor interaction graphs in Figure 11-41 (page 492), where x is the controllable factor and z is the noise factor. In Figure 11-41*a*, there is no $x \times z$ interaction; therefore, there is no setting for the controllable variable x that will affect the variability transmitted to the response by the variability in z. However, in Figure 11-41*b*, there is a strong $x \times z$ interaction. Note that when x is set to its low level, there is much less variability in the response variable than when x is at the high level. Thus, unless there is at least one controllable factor $\times$ noise factor interaction, there is no robust design problem. As we will see in the next section, focusing on identifying and modeling these interactions is one of the keys to a more efficient and effective approach to RPD.

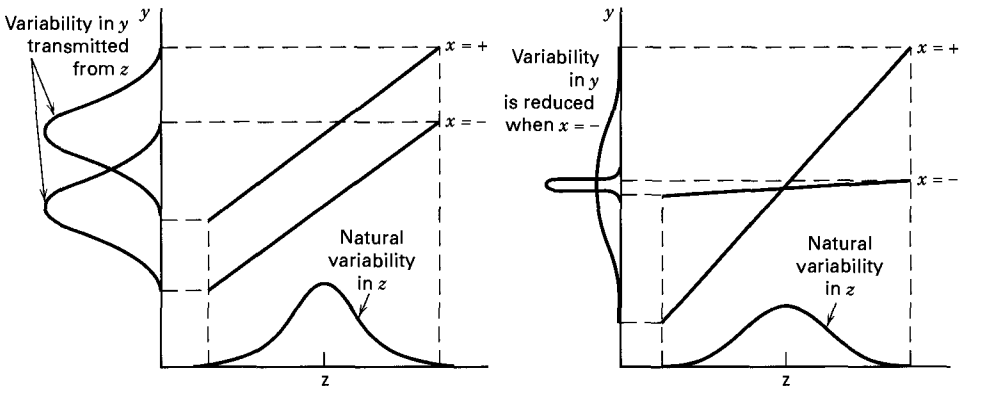


Figure 11-41 The role of the control × noise interaction in robust design.

11-7.2 The Response Surface Approach to Robust Design

As noted in the previous section, interactions between controllable and noise factors are the key to a robust design problem. Therefore, it is logical to use a **model** for the response that includes both controllable and noise factors and their interactions. To illustrate, suppose that we have two controllable factors x_1 and x_2 and a single noise factor z_1. We assume that both control and noise factors are expressed as the usual coded variables (that is, they are centered at zero and have lower and upper limits at $\pm a$). If we wish to consider a first-order model involving the controllable variables, a logical model is

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \gamma_1 z_1 + \delta_{11} x_1 z_1 + \delta_{21} x_2 z_1 + \epsilon \quad (11\text{-}28)$$

Notice that this model has the main effects of both controllable factors their interaction, the main effect of the noise variable, and both interactions between the controllable and noise variables. This type of model, incorporating both controllable and noise variables, is often called a **response model**. Unless at least one of the regression coefficients δ_{11} and δ_{21} is nonzero, there will be no robust design problem.

An important advantage of the response model approach is that both the controllable factors and the noise factors can be placed in a single experimental design; that is, the inner and outer array structure of the Taguchi approach can be avoided. We usually call the design containing both controllable and noise factors a **combined array design**.

As mentioned previously, we assume that noise variables are random variables, although they are controllable for purposes of an experiment. Specifically, we assume that the noise variables are expressed in coded units, that they have expected value zero, variance σ_z^2, and if there are several noise variables, they have zero covariances. Under these assumptions, it is easy to find a model for the mean response just by taking the expected value of y in Equation 11-28. This yields

$$E_z(y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$$

where the z subscript on the expectation operator is a reminder to take expected value with respect to *both* random variables in Equation 11-28, z_1 *and* ϵ. To find a model for the variance of the response y, we use the **transmission of error approach**. First, expand

the response model Equation 11-28 in a first-order Taylor series around $z_1 = 0$. This gives

$$\begin{aligned} y &\cong y_{z=0} + \frac{dy}{dz_1}(z_1 - 0) + R + \epsilon \\ &\cong \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 \\ &\quad + (\gamma_1 + \delta_{11} x_1 + \delta_{21} x_2) z_1 + R + \epsilon \end{aligned}$$

where R is the remainder term in the Taylor series. As is the usual practice, we will ignore the remainder term. Now the variance of y can be obtained by applying the variance operator across this last expression (without R). The resulting variance model is

$$V_z(y) = \sigma_z^2(\gamma_1 + \delta_{11} x_1 + \delta_{21} x_2)^2 + \sigma^2$$

Once again, we have used the z subscript on the variance operator as a reminder that *both* z_1 *and* ϵ are random variables.

We have derived simple models for the mean and variance of the response variable of interest. Note the following:

1. The mean and variance models involve **only the controllable variables**. This means we can potentially set the controllable variables to achieve a target value of the mean and minimize the variability transmitted by the noise variable.
2. Although the variance model involves only the controllable variables, it also involves the *interaction regression coefficients* between the controllable and noise variables. This is how the noise variable influences the response.
3. The variance model is a **quadratic function** of the controllable variables.
4. The variance model (apart from σ^2) is just the square of the **slope** of the fitted response model in the direction of the noise variable.

To use these models operationally, we would

1. Perform an experiment and fit an appropriate response model, such as Equation 11-28
2. Replace the unknown regression coefficients in the mean and variance models with their least squares estimates from the response model and replace σ^2 in the variance model by the residual mean square found when fitting the response model
3. Optimize the mean and variance model using the standard multiple response optimization methods discussed in Section 11-3.4

It is very easy to generalize these results. Suppose that there are k controllable variables and r noise variables. We will write the general response model involving these variables as

$$y(\mathbf{x}, \mathbf{z}) = f(\mathbf{x}) + h(\mathbf{x}, \mathbf{z}) + \epsilon \tag{11-29}$$

where $f(\mathbf{x})$ is the portion of the model that involves only the controllable variables and $h(\mathbf{x}, \mathbf{z})$ are the terms involving the main effects of the noise factors and the interactions between the controllable and noise factors. Typically, the structure for $h(\mathbf{x}, \mathbf{z})$ is

$$h(\mathbf{x}, \mathbf{z}) = \sum_{i=1}^{r} \gamma_i z_i + \sum_{i=1}^{k} \sum_{j=1}^{r} \delta_{ij} x_i z_j$$

The structure for $f(\mathbf{x})$ will depend on what type of model for the controllable variables the experimenter thinks is appropriate. The logical choices are the first-order model with interaction and the second-order model. If we assume that the noise variables have mean zero, variance σ_z^2, and zero covariances, and that the noise variables and the random errors ϵ have zero covariances, then the mean model for the response is just

$$E_z[y(\mathbf{x}, \mathbf{z})] = f(\mathbf{x}) \tag{11-30}$$

and the variance model for the response is

$$V_z[y(\mathbf{x}, \mathbf{z})] = \sigma_z^2 \sum_{i=1}^{r} \left[\frac{\partial y(\mathbf{x}, \mathbf{z})}{\partial z_i} \right]^2 + \sigma^2 \tag{11-31}$$

Myers and Montgomery (1995) give a slightly more general form for Equation (11-31) based on applying a conditional variance operator directly to the response model.

EXAMPLE 11-6

To illustrate the foregoing procedure, reconsider Example 6-2 in which four factors were studied in a 2^4 factorial design to investigate their effect on the filtration rate of a chemical product. We will assume that factor A, temperature, is hard to control in the full-scale process, but it can be controlled during the experiment (which was performed in a pilot plant). The other three factors, pressure (B), concentration (C), and stirring rate (D), are easy to control. Thus the noise factor z_1 is temperature, and the controllable variables x_1, x_2, and x_3 are pressure, concentration, and stirring rate, respectively. Because both the controllable factors and the noise factor are in the same design, the 2^4 factorial design used in this experiment is an example of a **combined array design**.

Using the results from Example 6-2, the response model is

$$\begin{aligned}\hat{y}(\mathbf{x}, z_1) &= 70.06 + \left(\frac{21.625}{2}\right) z_1 + \left(\frac{9.875}{2}\right) x_2 + \left(\frac{14.625}{2}\right) x_3 \\ &\quad - \left(\frac{18.125}{2}\right) x_2 z_1 + \left(\frac{16.625}{2}\right) x_3 z_1 \\ &= 70.06 + 10.81 z_1 + 4.94 x_2 + 7.31 x_3 - 9.06 x_2 z_1 + 8.31 x_3 z_1\end{aligned}$$

Using Equations (11-30) and (11-31), we can find the mean and variance models as

$$E_z[y(\mathbf{x}, z_1)] = 70.06 + 4.94 x_2 + 7.31 x_3$$

and

$$\begin{aligned}V_z[y(\mathbf{x}, z_1)] &= \sigma_z^2 (10.81 - 9.06 x_2 + 8.31 x_3)^2 + \sigma^2 \\ &= \sigma_z^2 (116.91 + 82.08 x_2^2 + 69.06 x_3^2 - 195.88 x_2 \\ &\quad + 179.66 x_3 - 150.58 x_2 x_3) + \sigma^2\end{aligned}$$

respectively. Now assume that the low and high levels of the noise variable temperature have been run at one standard deviation either side of its typical or average value, so that $\sigma_z^2 = 1$, and use $\hat{\sigma}^2 = 19.51$ (this is the residual mean square obtained by fitting the response model). Therefore, the variance model becomes

$$V_z[y(\mathbf{x}, z_1)] = 136.42 - 195.88 x_2 + 179.66 x_3 - 150.58 x_2 x_3 + 82.08 x_2^2 + 69.06 x_3^2$$

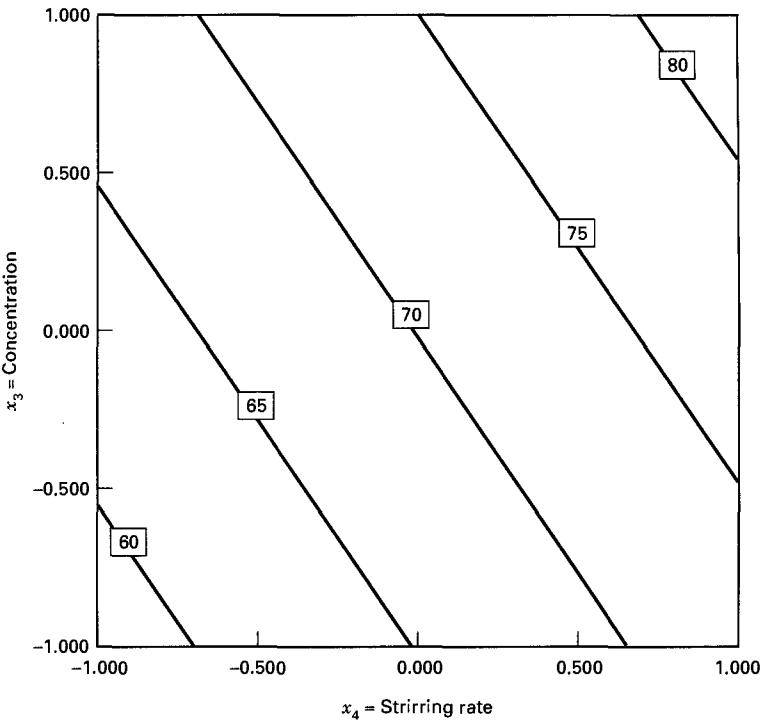
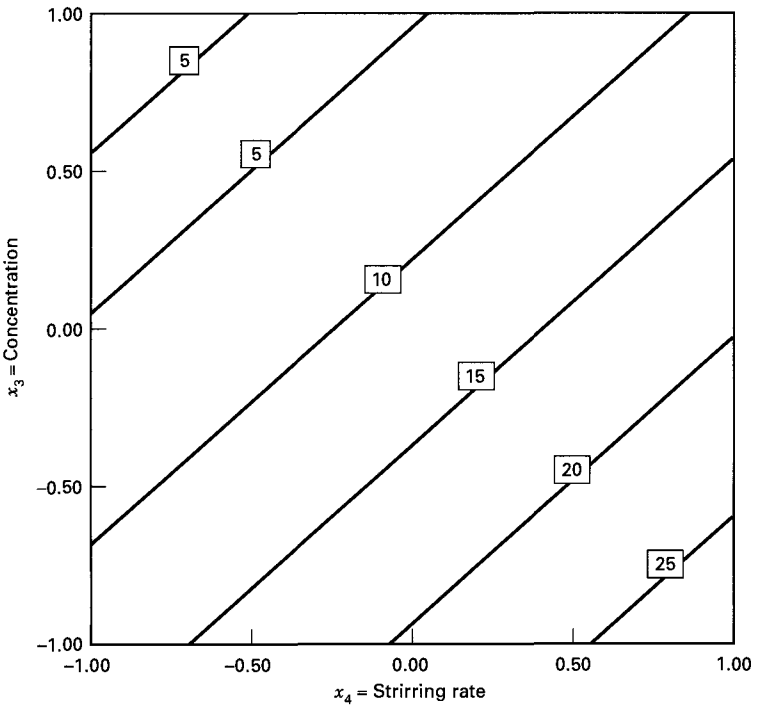


Figure 11-42 Contours of constant mean filtration rate, Example 11-6, with z_1 = temperature = 0.

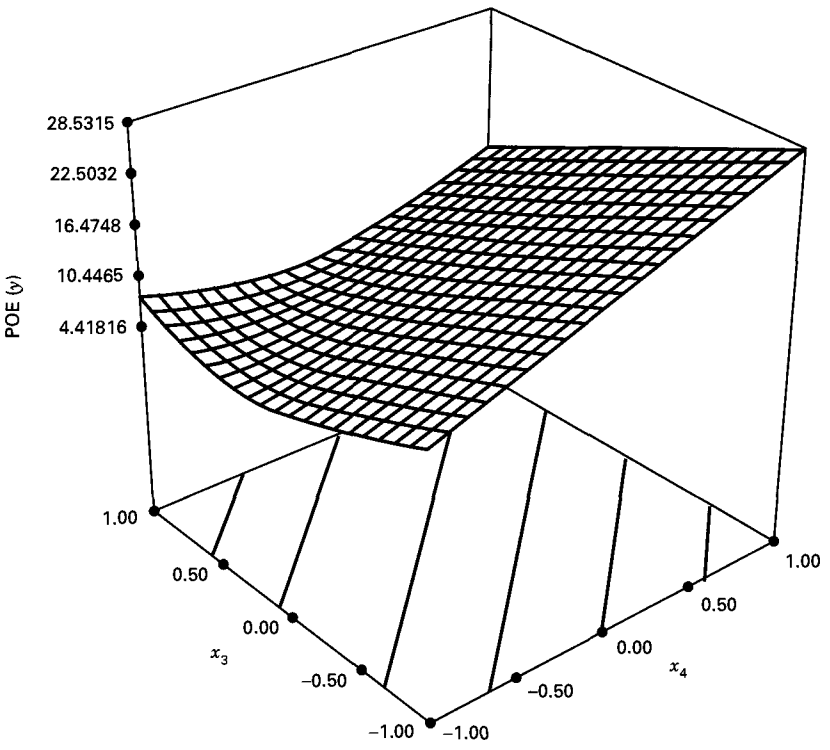
Figure 11-42 presents a contour plot from the Design-Expert software package of the response contours from the mean model. To construct this plot, we held the noise factor (temperature) at zero and the nonsignificant controllable factor (pressure) at zero. Notice that mean filtration rate increases as both concentration and stirring rate increase. Design-Expert will also construct plots automatically of the **square root** of the variance contours, which it labels **propagation of error**, or **POE**. Obviously, the POE is just the standard deviation of the transmitted variability in the response as a function of the controllable variables. Figure 11-43 (page 496) shows a contour plot and a three-dimensional response surface plot of the POE, obtained from Design-Expert (in this plot the noise variable is held constant at zero, as explained previously).

Suppose that the experimenter wants to maintain a mean filtration rate about 75 and minimize the variability around this value. Figure 11-44 (page 497) shows an overlay plot of the contours of mean filtration rate and the POE as a function of concentration and stirring rate, the significant controllable variables. To achieve the desired objectives, it will be necessary to hold concentration at the high level and stirring rate very near the middle level.

Example 11-6 illustrates the use of a first-order model with interaction as the model for the controllable factors, $f(\mathbf{x})$. We now present an example adapted from Montgomery (1999) that involves a second-order model.



(*a*) Contour plot



(*b*) Response surface plot

Figure 11-43 Contour plot and response surface of propagation of error for Example 11-6, with z_1 = temperature = 0.

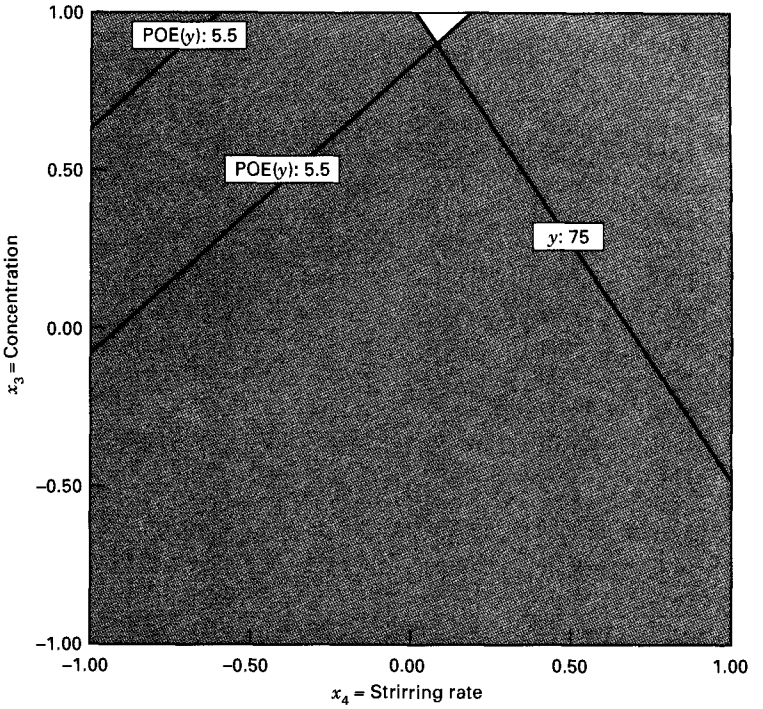


Figure 11-44 Overlay plot of mean and POE contours for filtration rate, Example 11-6, with z_1 temperature = 0.

EXAMPLE 11-7

An experiment was run in a semiconductor manufacturing facility involving two controllable variables and three noise variables. The combined array design used by the experimenters is shown in Table 11-23 on the next page. The design is a 23-run variation of a central composite design that was created by starting with a standard CCD for five factors (the cube portion is a 2^{5-1}) and deleting the axial runs associated with the three noise variables. This design will support a response model that has a second-order model in the controllable variables, the main effects of the three noise variables, and the interactions between the control and noise factors. The fitted response model is

$$\begin{aligned}\hat{y}(\mathbf{x}, \mathbf{z}) = {} & 30.37 - 2.92x_1 - 4.13x_2 + 2.60x_1^2 + 2.18x_2^2 + 2.87x_1x_2 \\ & + 2.73z_1 - 2.33z_2 + 2.33z_3 - 0.27x_1z_1 + 0.89x_1z_2 + 2.58x_1z_3 \\ & + 2.01x_2z_1 - 1.43x_2z_2 + 1.56x_2z_3\end{aligned}$$

The mean and variance models are

$$E_{\mathbf{z}}[y(\mathbf{x}, \mathbf{z})] = 30.37 - 2.92x_1 - 4.13x_2 + 2.60x_1^2 + 2.18x_2^2 + 2.87x_1x_2$$

and

$$V_{\mathbf{z}}[y(\mathbf{x}, \mathbf{z})] = 19.26 + 3.20x_1 + 12.45x_2 + 7.52x_1^2 + 8.52x_2^2 + 2.21x_1x_2$$

where we have substituted parameter estimates from the fitted response model into the equations for the mean and variance models and, as in the previous example, assumed that $\sigma_{\mathbf{z}}^2 = 1$. Figures 11-45 and 11-46 (pages 498–499) (from Design-Expert) present contour plots of the process mean and POE (remember POE is the square root of the variance response surface) generated from these models.

Table 11-23 Combined Array Experiment with Two Controllable Variables and Three Noise Variables, Example 11-7

Run Number	x_1	x_2	z_1	z_2	z_3	y
1	−1.00	−1.00	−1.00	−1.00	1.00	44.2
2	1.00	−1.00	−1.00	−1.00	−1.00	30.0
3	−1.00	1.00	−1.00	−1.00	−1.00	30.0
4	1.00	1.00	−1.00	−1.00	1.00	35.4
5	−1.00	−1.00	1.00	−1.00	−1.00	49.8
6	1.00	−1.00	1.00	−1.00	1.00	36.3
7	−1.00	1.00	1.00	−1.00	1.00	41.3
8	1.00	1.00	1.00	−1.00	−1.00	31.4
9	−1.00	−1.00	−1.00	1.00	−1.00	43.5
10	1.00	−1.00	−1.00	1.00	1.00	36.1
11	−1.00	1.00	−1.00	1.00	1.00	22.7
12	1.00	1.00	−1.00	1.00	−1.00	16.0
13	−1.00	−1.00	1.00	1.00	1.00	43.2
14	1.00	−1.00	1.00	1.00	−1.00	30.3
15	−1.00	1.00	1.00	1.00	−1.00	30.1
16	1.00	1.00	1.00	1.00	1.00	39.2
17	−2.00	0.00	0.00	0.00	0.00	46.1
18	2.00	0.00	0.00	0.00	0.00	36.1
19	0.00	−2.00	0.00	0.00	0.00	47.4
20	0.00	2.00	0.00	0.00	0.00	31.5
21	0.00	0.00	0.00	0.00	0.00	30.8
22	0.00	0.00	0.00	0.00	0.00	30.7
23	0.00	0.00	0.00	0.00	0.00	31.0

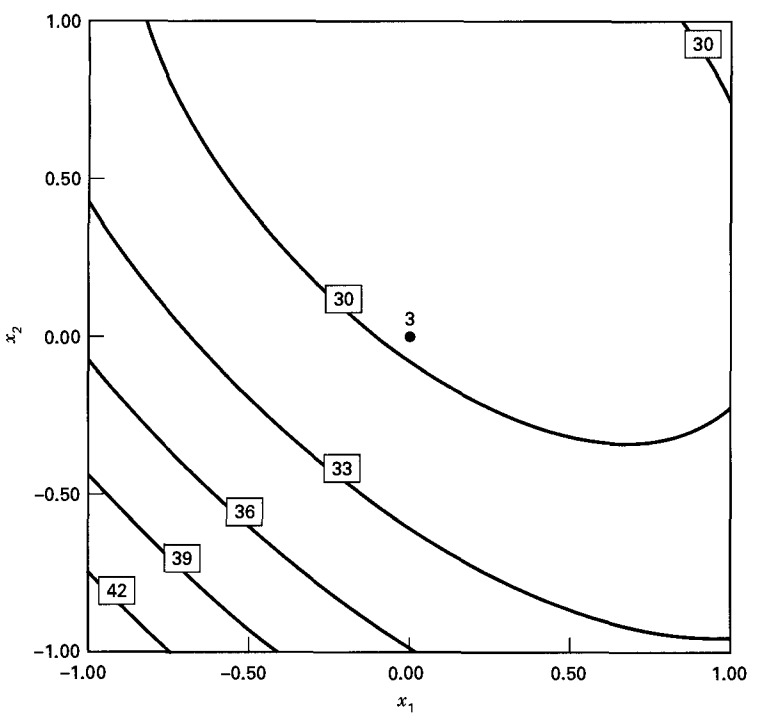


Figure 11-45 Contour plot of the mean model, Example 11-7.

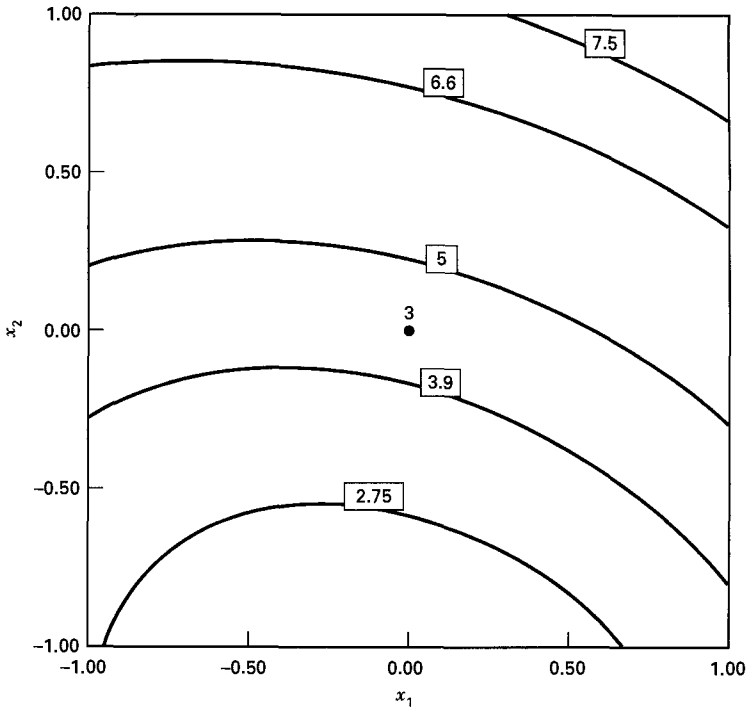


Figure 11-46 Contour plot of the POE, Example 11-7.

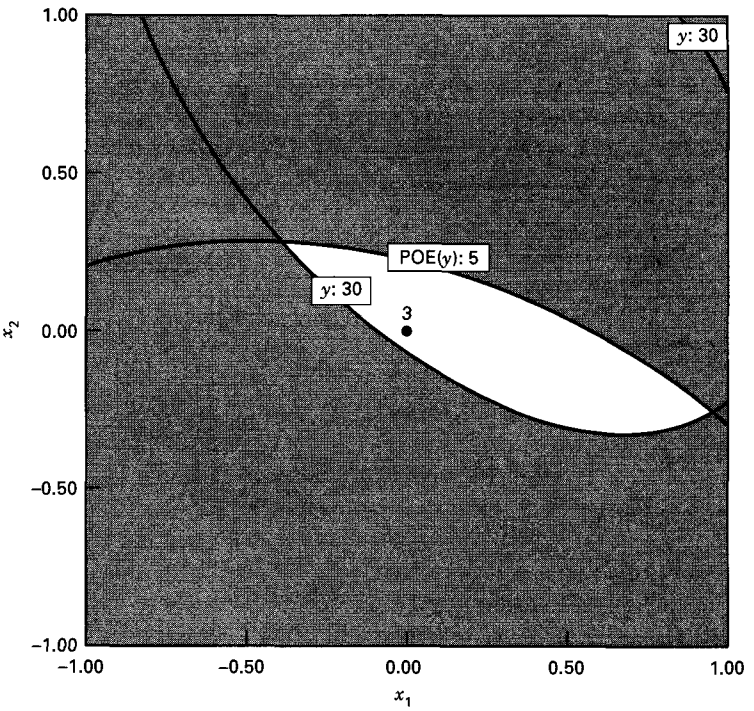


Figure 11-47 Overlay of the mean and POE contours for Example 11-7, with the open region indicating satisfactory operating conditions for process mean and variance.

In this problem it is desirable to keep the process mean below 30. From inspection of Figures 11-45 and 11-46 it is clear that some trade-off will be necessary if we wish to make the process variance small. Because there are only two controllable variables, a logical way to accomplish this trade-off is to overlay the contours of constant mean response and constant variance, as shown in Figure 11-47 on the previous page. This plot shows the contours for which the process mean is less than or equal to 30 and the process standard deviation is less than or equal to 5. The region bounded by these contours would represent a typical operating region of low mean response and low process variance.

11-8 PROBLEMS

11-1. A chemical plant produces oxygen by liquifying air and separating it into its component gases by fractional distillation. The purity of the oxygen is a function of the main condenser temperature and the pressure ratio between the upper and lower columns. Current operating conditions are temperature (ξ_1) = −220°C and pressure ratio (ξ_2) = 1.2. Using the following data, find the path of steepest ascent:

Temperature (ξ_1)	Pressure Ratio (ξ_2)	Purity
−225	1.1	82.8
−225	1.3	83.5
−215	1.1	84.7
−215	1.3	85.0
−220	1.2	84.1
−220	1.2	84.5
−220	1.2	83.9
−220	1.2	84.3

11-2. An industrial engineer has developed a computer simulation model of a two-item inventory system. The decision variables are the order quantity and the reorder point for each item. The response to be minimized is total inventory cost. The simulation model is used to produce the data shown in the following table. Identify the experimental design. Find the path of steepest descent.

Item 1		Item 2		
Order Quantity (ξ_1)	Reorder Point (ξ_2)	Order Quantity (ξ_3)	Reorder Point (ξ_4)	Total Cost
100	25	250	40	625
140	45	250	40	670
140	25	300	40	663
140	25	250	80	654
100	45	300	40	648
100	45	250	80	634
100	25	300	80	692
140	45	300	80	686
120	35	275	60	680
120	35	275	60	674
120	35	275	60	681

11-3. Verify that the following design is a simplex. Fit the first-order model, and find the path of steepest ascent.

x_1	x_2	x_3	y
0	$\sqrt{2}$	-1	18.5
$-\sqrt{2}$	0	1	19.8
0	$-\sqrt{2}$	-1	17.4
$\sqrt{2}$	0	1	22.5

11-4. For the first-order model

$$\hat{y} = 60 + 1.5x_1 - 0.8x_2 + 2.0x_3$$

find the path of steepest ascent. The variables are coded as $-1 \leq x_i \leq 1$.

11-5. The region of experimentation for three factors are time ($40 \leq T_1 \leq 80$ min), temperature ($200 \leq T_2 \leq 300$°C), and pressure ($20 \leq P \leq 50$ psig). A first-order model in coded variables has been fit to yield data from a 2^3 design. The model is

$$\hat{y} = 30 + 5x_1 + 2.5x_2 + 3.5x_3$$

Is the point $T_1 = 85$, $T_2 = 325$, $P = 60$ on the path of steepest ascent?

11-6. The region of experimentation for two factors are temperature ($100 \leq T \leq 300$°F) and catalyst feed rate ($10 \leq C \leq 30$ lb/in). A first-order model in the usual ± 1 coded variables has been fit to a molecular weight response, yielding the following model:

$$\hat{y} = 2000 + 125x_1 + 40x_2$$

(a) Find the path of steepest ascent.

(b) It is desired to move to a region where molecular weights are above 2500. Based on the information you have from experimentation in this region, about how many steps along the path of steepest ascent might be required to move to the region of interest?

11-7. The path of steepest ascent is usually computed assuming that the model is truly first-order; that is, there is no interaction. However, even if there is interaction, steepest ascent ignoring the interaction still usually produces good results. To illustrate, suppose that we have fit the model

$$\hat{y} = 20 + 5x_1 - 8x_2 + 3x_1x_2$$

using coded variables ($-1 \leq x_i \leq +1$).

(a) Draw the path of steepest ascent that you would obtain if the interaction were ignored.

(b) Draw the path of steepest ascent that you would obtain with the interaction included in the model. Compare this with the path found in part (a).

11-8. The data shown in the following table were collected in an experiment to optimize crystal growth as a function of three variables x_1, x_2, and x_3. Large values of y (yield in grams) are desirable. Fit a second-order model and analyze the fitted surface. Under what set of conditions is maximum growth achieved?

x_1	x_2	x_3	y
−1	−1	−1	66
−1	−1	1	70
−1	1	−1	78
−1	1	1	60
1	−1	−1	80
1	−1	1	70
1	1	−1	100
1	1	1	75
−1.682	0	0	100
1.682	0	0	80
0	−1.682	0	68
0	1.682	0	63
0	0	−1.682	65
0	0	1.682	82
0	0	0	113
0	0	0	100
0	0	0	118
0	0	0	88
0	0	0	100
0	0	0	85

11-9. The following data were collected by a chemical engineer. The response y is filtration time, x_1 is temperature, and x_2 is pressure. Fit a second-order model.

x_1	x_2	y
−1	−1	54
−1	1	45
1	−1	32
1	1	47
−1.414	0	50
1.414	0	53
0	−1.414	47
0	1.414	51
0	0	41
0	0	39
0	0	44
0	0	42
0	0	40

(a) What operating conditions would you recommend if the objective is to minimize the filtration time?

(b) What operating conditions would you recommend if the objective is to operate the process at a mean filtration rate very close to 46?

11-10. The hexagon design that follows is used in an experiment that has the objective of fitting a second-order model:

x_1	x_2	y
1	0	68
0.5	$\sqrt{0.75}$	74
−0.5	$\sqrt{0.75}$	65
−1	0	60
−0.5	$-\sqrt{0.75}$	63
0.5	$-\sqrt{0.75}$	70
0	0	58
0	0	60
0	0	57
0	0	55
0	0	69

(a) Fit the second-order model.
(b) Perform the canonical analysis. What type of surface has been found?
(c) What operating conditions on x_1 and x_2 lead to the stationary point?
(d) Where would you run this process if the objective is to obtain a response that is as close to 65 as possible?

11-11. An experimenter has run a Box–Behnken design and has obtained the results below, where the response variable is the viscosity of a polymer:

Level	Temp.	Agitation Rate	Pressure	x_1	x_2	x_3
High	200	10.0	25	+1	+1	+1
Middle	175	7.5	20	0	0	0
Low	150	5.0	15	−1	−1	−1

Run	x_1	x_2	x_3	y_1
1	−1	−1	0	535
2	+1	−1	0	580
3	−1	+1	0	596
4	+1	+1	0	563
5	−1	0	−1	645
6	+1	0	−1	458
7	−1	0	+1	350
8	+1	0	+1	600
9	0	−1	−1	595
10	0	+1	−1	648
11	0	−1	+1	532
12	0	+1	+1	656
13	0	0	0	653
14	0	0	0	599
15	0	0	0	620

(a) Fit the second-order model.
(b) Perform the canonical analysis. What type of surface has been found?

(c) What operating conditions on x_1, x_2, and x_3 lead to the stationary point?
(d) What operating conditions would you recommend if it is important to obtain a viscosity that is as close to 600 as possible?

11-12. Consider the three-variable central composite design shown below. Analyze the data and draw conclusions, assuming that we wish to maximize conversion (y_1) with activity (y_2) between 55 and 60.

Run	Time (min)	Temperature (°C)	Catalyst (%)	Conversion (%) y_1	Activity y_2
1	−1.000	−1.000	−1.000	74.00	53.20
2	1.000	−1.000	−1.000	51.00	62.90
3	−1.000	1.000	−1.000	88.00	53.40
4	1.000	1.000	−1.000	70.00	62.60
5	−1.000	−1.000	1.000	71.00	57.30
6	1.000	−1.000	1.000	90.00	67.90
7	−1.000	1.000	1.000	66.00	59.80
8	1.000	1.000	1.000	97.00	67.80
9	0.000	0.000	0.000	81.00	59.20
10	0.000	0.000	0.000	75.00	60.40
11	0.000	0.000	0.000	76.00	59.10
12	0.000	0.000	0.000	83.00	60.60
13	−1.682	0.000	0.000	76.00	59.10
14	1.682	0.000	0.000	79.00	65.90
15	0.000	−1.682	0.000	85.00	60.00
16	0.000	1.682	0.000	97.00	60.70
17	0.000	0.000	−1.682	55.00	57.40
18	0.000	0.000	1.682	81.00	63.20
19	0.000	0.000	0.000	80.00	60.80
20	0.000	0.000	0.000	91.00	58.90

11-13. A manufacturer of cutting tools has developed two empirical equations for tool life in hours (y_1) and for tool cost in dollars (y_2). Both models are linear functions of steel hardness (x_1) and manufacturing time (x_2). The two equations are

$$\hat{y}_1 = 10 + 5x_1 + 2x_2$$
$$\hat{y}_2 = 23 + 3x_1 + 4x_2$$

and both equations are valid over the range $-1.5 \leq x_i \leq 1.5$. Unit tool cost must be below \$27.50 and life must exceed 12 hours for the product to be competitive. Is there a feasible set of operating conditions for this process? Where would you recommend that the process be run?

11-14. A central composite design is run in a chemical vapor deposition process, resulting in the experimental data shown on the next page. Four experimental units were processed simultaneously on each run of the design, and the responses are the mean and variance of thickness, computed across the four units.

x_1	x_2	$\bar{y}$	s^2
−1	−1	360.6	6.689
1	−1	445.2	14.230
−1	1	412.1	7.088
1	1	601.7	8.586
1.414	0	518.0	13.130
−1.414	0	411.4	6.644
0	1.414	497.6	7.649
0	−1.414	397.6	11.740
0	0	530.6	7.836
0	0	495.4	9.306
0	0	510.2	7.956
0	0	487.3	9.127

(a) Fit a model to the mean response. Analyze the residuals.
(b) Fit a model to the variance response. Analyze the residuals.
(c) Fit a model to $\ln(s^2)$. Is this model superior to the one you found in part (b)?
(d) Suppose you want the mean thickness to be in the interval 450 ± 25. Find a set of operating conditions that achieve this objective and simultaneously minimize the variance.
(e) Discuss the variance minimization aspects of part (d). Have you minimized the *total* process variance?

11-15. Verify that an orthogonal first-order design is also first-order rotatable.

11-16. Show that augmenting a 2^k design with n_c center points does not affect the estimates of the β_i ($i = 1, 2, \ldots, k$) but that the estimate of the intercept β_0 is the average of all $2^k + n_c$ observations.

11-17. ***The rotatable central composite design.*** It can be shown that a second-order design is rotatable if $\Sigma_{u=1}^{n} x_{iu}^{a} x_{ju}^{b} = 0$ if a or b (or both) are odd and if $\Sigma_{u=1}^{n} x_{iu}^{4} = 3\Sigma_{u=1}^{n} x_{iu}^{2} x_{ju}^{2}$. Show that for the central composite design these conditions lead to $\alpha = (n_F)^{1/4}$ for rotatability, where n_F is the number of points in the factorial portion.

11-18. Verify that the central composite design shown below blocks orthogonally:

Block 1			Block 2			Block 3		
x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
0	0	0	0	0	0	−1.633	0	0
0	0	0	0	0	0	1.633	0	0
1	1	1	1	1	−1	0	−1.633	0
1	−1	−1	1	−1	1	0	1.633	0
−1	−1	1	−1	1	1	0	0	−1.633
−1	1	−1	−1	−1	−1	0	0	1.633
						0	0	0
						0	0	0

11-19. ***Blocking in the central composite design.*** Consider a central composite design for $k = 4$ variables in two blocks. Can a rotatable design always be found that blocks orthogonally?

11-20. How could a hexagon design be run in two orthogonal blocks?

11-21. Yield during the first four cycles of a chemical process is shown in the following table. The variables are percentage of concentration (x_1) at levels 30, 31, and 32 and temperature (x_2) at 140, 142, and 144°F. Analyze by EVOP methods.

	Conditions				
Cycle	(1)	(2)	(3)	(4)	(5)
1	60.7	59.8	60.2	64.2	57.5
2	59.1	62.8	62.5	64.6	58.3
3	56.6	59.1	59.0	62.3	61.1
4	60.5	59.8	64.5	61.0	60.1

11-22. Suppose that we approximate a response surface with a model of order d_1, such as $\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \boldsymbol{\epsilon}$, when the true surface is described by a model of order $d_2 > d_1$; that is, $E(\mathbf{y}) = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_1\boldsymbol{\beta}_2$.

(a) Show that the regression coefficients are biased, that is, that $E(\hat{\boldsymbol{\beta}}_1) = \boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2$, where $\mathbf{A} = (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2$. $\mathbf{A}$ is usually called the alias matrix.

(b) If $d_1 = 1$ and $d_2 = 2$, and a full 2^k is used to fit the model, use the result in part (a) to determine the alias structure.

(c) If $d_1 = 1$, $d_2 = 2$, and $k = 3$, find the alias structure assuming that a 2^{3-1} design is used to fit the model.

(d) If $d_1 = 1$, $d_2 = 2$, $k = 3$, and the simplex design in Problem 11-3 is used to fit the model, determine the alias structure and compare the results with part (c).

11-23. In an article ("Let's All Beware the Latin Square," *Quality Engineering*, Vol. 1, 1989, pp. 453–465), J. S. Hunter illustrates some of the problems associated with 3^{k-p} fractional factorial designs. Factor A is the amount of ethanol added to a standard fuel and factor B represents the air/fuel ratio. The response variable is carbon monoxide (CO) emission in g/m^3. The design is shown below:

Design				Observations	
A	B	x_1	x_2	y	
0	0	−1	−1	66	62
1	0	0	−1	78	81
2	0	+1	−1	90	94
0	1	−1	0	72	67
1	1	0	0	80	81
2	1	+1	0	75	78
0	2	−1	+1	68	66
1	2	0	+1	66	69
2	2	+1	+1	60	58

Notice that we have used the notation system of 0, 1, and 2 to represent the low, medium, and high levels for the factors. We have also used a "geometric notation" of −1, 0, and +1. Each run in the design is replicated twice.

(a) Verify that the second-order model

$$\hat{y} = 78.5 + 4.5x_1 - 7.0x_2 - 4.5x_1^2 - 4.0x_2^2 - 9.0x_1x_2$$

is a reasonable model for this experiment. Sketch the CO concentration contours in the x_1, x_2 space.

(b) Now suppose that instead of only two factors, we had used *four* factors in a 3^{4-2} fractional factorial design and obtained *exactly* the same data as in part (a). The design would be as follows:

Design								Observations	
A	B	C	D	x_1	x_2	x_3	x_4	y	
0	0	0	0	−1	−1	−1	−1	66	62
1	0	1	1	0	−1	0	0	78	81
2	0	2	2	+1	−1	+1	+1	90	94
0	1	2	1	−1	0	+1	0	72	67
1	1	0	2	0	0	−1	+1	80	81
2	1	1	0	+1	0	0	−1	75	78
0	2	1	2	−1	+1	0	+1	68	66
1	2	2	0	0	+1	+1	−1	66	69
2	2	0	1	+1	+1	−1	0	60	58

Confirm that this design is an L_9 orthogonal array.

(c) Calculate the marginal averages of the CO response at each level of the four factors A, B, C, and D. Construct plots of these marginal averages and interpret the results. Do factors C and D appear to have strong effects? Do these factors *really* have any effect on CO emission? Why is their apparent effect strong?

(d) The design in part (b) allows the model

$$y = \beta_0 + \sum_{i=1}^{4} \beta_i x_i + \sum_{i=1}^{4} \beta_{ii} x_i^2 + \epsilon$$

to be fitted. Suppose that the *true* model is

$$y = \beta_0 + \sum_{i=1}^{4} \beta_i x_i + \sum_{i=1}^{4} \beta_{ii} x_i^2 + \sum\sum_{i<j} \beta_{ij} x_i x_j = \epsilon$$

Show that if $\hat{\beta}_j$ represents the least squares estimates of the coefficients in the fitted model, then

$$\begin{aligned}
E(\hat{\beta}_0) &= \beta_0 - \beta_{13} - \beta_{14} - \beta_{34} \\
E(\hat{\beta}_1) &= \beta_1 - (\beta_{23} + \beta_{24})/2 \\
E(\hat{\beta}_2) &= \beta_2 - (\beta_{13} + \beta_{14} + \beta_{34})/2 \\
E(\hat{\beta}_3) &= \beta_3 - (\beta_{12} + \beta_{24})/2 \\
E(\hat{\beta}_4) &= \beta_4 - (\beta_{12} + \beta_{23})/2 \\
E(\hat{\beta}_{11}) &= \beta_{11} - (\beta_{23} - \beta_{24})/2 \\
E(\hat{\beta}_{22}) &= \beta_{22} + (\beta_{13} + \beta_{14} + \beta_{34})/2 \\
E(\hat{\beta}_{33}) &= \beta_{33} - (\beta_{24} - \beta_{12})/2 + \beta_{14} \\
E(\hat{\beta}_{44}) &= \beta_{44} - (\beta_{12} - \beta_{23})/2 + \beta_{13}
\end{aligned}$$

Does this help explain the strong effects for factors C and D observed graphically in part (c)?

11-24. Suppose that you need to design an experiment to fit a quadratic model over the region $-1 \leq x_i \leq +1$, $i = 1, 2$ subject to the constraint $x_1 + x_2 \leq 1$. If the constraint is violated,

the process will not work properly. You can afford to make no more than $n = 12$ runs. Set up the following designs:

(a) An "inscribed" CCD with center point at $x_1 = x_2 = 0$.
(b) An "inscribed" 3^2 factorial with center point at $x_1 = x_2 = -0.25$.
(c) A D-optimal design.
(d) A modified D-optimal design that is identical to the one in part (c), but with all replicate runs at the design center.
(e) Evaluate the $|(\mathbf{X}'\mathbf{X})^{-1}|$ criterion for each design.
(f) Evaluate the D-efficiency for each design relative to the D-optimal design in part (c).
(g) Which design would you prefer? Why?

11-25. Consider a 2^3 design for fitting a first-order model.
(a) Evaluate the D-criterion $|(\mathbf{X}'\mathbf{X})^{-1}|$ for this design.
(b) Evaluate the A-criterion $\text{tr}(\mathbf{X}'\mathbf{X})^{-1}$ for this design.
(c) Find the maximum scaled prediction variance for this design. Is this design G-optimal?

11-26. Repeat Problem 11-25 using a first-order model with the two-factor interactions.

11-27. A chemical engineer wishes to fit a calibration curve for a new procedure used to measure the concentration of a particular ingredient in a product manufactured in his facility. Twelve samples can be prepared, having known concentration. The engineer wants to build a model for the measured concentrations. He suspects that a linear calibration curve will be adequate to model the measured concentration as a function of the known concentrations; that is, $y = \beta_0 + \beta_1 x + \epsilon$, where x is the actual concentration. Four experimental designs are under consideration. Design 1 consists of six runs at known concentration 1 and six runs at known concentration 10. Design 2 consists of four runs at concentrations 1, 5.5, and 10. Design 3 consists of three runs at concentration 1, 4, 7, and 10. Finally, design 4 consists of three runs at concentrations 1, and 10 and six runs at concentration 5.5.
(a) Plot the scaled variance of prediction for all four designs on the same graph over the concentration range $1 \leq x \leq 10$. Which design would be preferable?
(b) For each design calculate the determinant of $(\mathbf{X}'\mathbf{X})^{-1}$. Which design would be preferred according to the D-criterion?
(c) Calculate the D-efficiency of each design relative to the "best" design that you found in part (b).
(d) For each design, calculate the average variance of prediction over the set of points given by $x = 1, 1.5, 2, 2.5, \ldots, 10$. Which design would you prefer according to the V-criterion?
(e) Calculate the V-efficiency of each design relative to the best design that you found in part (d).
(f) What is the G-efficiency of each design?

11-28. Rework problem 11-27 assuming that the model the engineer wishes to fit is a quadratic. Obviously, only designs 2, 3, and 4 can now be considered.

11-29. An experimenter wishes to run a three-component mixture experiment. The constraints in the component proportions are as follows:

$$0.2 \leq x_1 \leq 0.4$$
$$0.1 \leq x_2 \leq 0.3$$
$$0.4 \leq x_2 \leq 0.7$$

(a) Set up an experiment to fit a quadratic mixture model. Use $n = 14$ runs, with four replicates. Use the D-criterion.
(b) Draw the experimental region.

(c) Set up an experiment to fit a quadratic mixture model with $n = 12$ runs, assuming that three of these runs are replicates. Use the D-criterion.

(d) Comment on the two designs you have found.

11-30. Myers and Montgomery (1995) describe a gasoline blending experiment involving three mixture components. There are no constraints on the mixture proportions, and the following 10-run design is used:

Design Point	x_1	x_2	x_3	y, mi/gal
1	1	0	0	24.5, 25.1
2	0	1	0	24.8, 23.9
3	0	0	1	22.7, 23.6
4	$\frac{1}{2}$	$\frac{1}{2}$	0	25.1
5	$\frac{1}{2}$	0	$\frac{1}{2}$	24.3
6	0	$\frac{1}{2}$	$\frac{1}{2}$	23.5
7	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	24.8, 24.1
8	$\frac{2}{3}$	$\frac{1}{6}$	$\frac{1}{6}$	24.2
9	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$	23.9
10	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{2}{3}$	23.7

(a) What type of design did the experimenters use?

(b) Fit a quadratic mixture model to the data. Is this model adequate?

(c) Plot the response surface contours. What blend would you recommend to maximize the miles per gallon?

11-31. Consider the bottle-filling experiment in Example 6-1. Suppose that the percentage of carbonation (A) is a noise variable (in coded units $\sigma_z^2 = 1$).

(a) Fit the response model to these data. Is there a robust design problem?

(b) Find the mean model and either the variance model or the POE.

(c) Find a set of conditions that result in mean fill deviation as close to zero as possible with minimum transmitted variance.

11-32. Consider the experiment in Problem 11-12. Suppose that temperature is a noise variable ($\sigma_z^2 = 1$ in coded units). Fit response models for both responses. Is there a robust design problem with respect to both responses? Find a set of conditions that maximize conversion with activity between 55 and 60 and that minimize the variability transmitted from temperature.

11-33. An experiment has been run in a process that applies a coating material to a wafer. Each run in the experiment produced a wafer, and the coating thickness was measured several times at different locations on the wafer. Then the mean y_1 and standard deviation y_2 of the thickness measurement was obtained. The data [adapted from Box and Draper (1987)] are shown in the table below:

Run	Speed	Pressure	Distance	Mean y_1	Std. Dev. y_2
1	−1.000	−1.000	−1.000	24.0	12.5
2	0.000	−1.000	−1.000	120.3	8.4
3	1.000	−1.000	−1.000	213.7	42.8
4	−1.000	0.000	−1.000	86.0	3.5
5	0.000	0.000	−1.000	136.6	80.4
6	1.000	0.000	−1.000	340.7	16.2
7	−1.000	1.000	−1.000	112.3	27.6

Run	Speed	Pressure	Distance	Mean y_1	Std. Dev. y_2
8	0.000	1.000	−1.000	256.3	4.6
9	1.000	1.000	−1.000	271.7	23.6
10	−1.000	−1.000	0.000	81.0	0.0
11	0.000	−1.000	0.000	101.7	17.7
12	1.000	−1.000	0.000	357.0	32.9
13	−1.000	0.000	0.000	171.3	15.0
14	0.000	0.000	0.000	372.0	0.0
15	1.000	0.000	0.000	501.7	92.5
16	−1.000	1.000	0.000	264.0	63.5
17	0.000	1.000	0.000	427.0	88.6
18	1.000	1.000	0.000	730.7	21.1
19	−1.000	−1.000	1.000	220.7	133.8
20	0.000	−1.000	1.000	239.7	23.5
21	1.000	−1.000	1.000	422.0	18.5
22	−1.000	0.000	1.000	199.0	29.4
23	0.000	0.000	1.000	485.3	44.7
24	1.000	0.000	1.000	673.7	158.2
25	−1.000	1.000	1.000	176.7	55.5
26	0.000	1.000	1.000	501.0	138.9
27	1.000	1.000	1.000	1010.0	142.4

(a) What type of design did the experimenters use? Is this a good choice of design for fitting a quadratic model?
(b) Build models of both responses.
(c) Find a set of optimum conditions that result in the mean as large as possible with the standard deviation less than 60.

11-34. ***A variation of Example 6-2.*** In Example 6-2 we found that one of the process variables (B = pressure) was not important. Dropping this variable produces two replicates of a 2^3 design. The data are shown below:

C	D	A (+)	A (−)	$\bar{y}$	s^2
−	−	45, 48	71, 65	57.75	121.19
+	−	68, 80	60, 65	68.25	72.25
−	+	43, 45	100, 104	73.00	1124.67
+	+	75, 70	86, 96	81.75	134.92

Assume that C and D are controllable factors and that A is a noise variable.
(a) Fit a model to the mean response.
(b) Fit a model to the $ln(s^2)$ response.
(c) Find operating conditions that result in the mean filtration rate response exceeding 75 with minimum variance.
(d) Compare your results with those from Example 11-6, which used the transmission of error approach. How similar are the two answers?

12 Experiments with Random Factors

Throughout most of this book we have assumed that the factors in an experiment were **fixed factors**, that is, the levels of the factors used by the experimenter were the specific levels of interest. The implication of this, of course, is that the statistical inferences made about these factors is confined to the specific levels studied. That is, if three material types are investigated as in the battery life experiment of Example 5-1, our conclusions are valid only about those specific material types. A variation of this occurs when the factor or factors are **quantitative**. In these situations, we often use a regression model relating the response to the factors to predict the response over the region spanned by the factor levels used in the experimental design. Several examples of this were presented in Chapters 5 through 9. In general, with a fixed effect, we say that the **inference space** of the experiment is the specific set of factor levels investigated.

In some experimental situations, the factor levels are chosen at random from a larger population of possible levels, and the experimenter wishes to draw conclusions about the entire population of levels, not just those that were used in the experimental design. In this situation the factor is said to be a **random factor**. We begin with a simple situation, a single-factor experiment where the factor is random and use this to introduce the **random effects model** for the analysis of variance and **components of variance**. Random factors also occur regularly in factorial experiments as well as in other types of experiments. In this chapter we focus on methods for the design and analysis of factorial experiments with random factors. In Chapter 13 we will present nested and split-plot designs, two situations where random factors are frequently encountered in practice.

12-1 THE RANDOM EFFECTS MODEL

An experimenter is frequently interested in a factor that has a large number of possible levels. If the experimenter randomly selects a of these levels from the population of factor levels, then we say that the factor is **random**. Because the levels of the factor actually used in the experiment were chosen randomly, inferences are made about the entire population of factor levels. We assume that the population of factor levels is either of infinite size or is large enough to be considered infinite. Situations in which the pop-

ulation of factor levels is small enough to employ a finite population approach are not encountered frequently. Refer to Bennett and Franklin (1954) and Searle and Fawcett (1970) for a discussion of the finite population case.

The linear statistical model is

$$y_{ij} = \mu + \tau_i + \epsilon_{ij} \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, n \end{cases} \tag{12-1}$$

where both τ_i and ϵ_{ij} are random variables. If τ_i has variance σ_τ^2 and is independent of ϵ_{ij}, the variance of any observation is

$$V(y_{ij}) = \sigma_\tau^2 + \sigma^2$$

The variances σ_τ^2 and σ^2 are called **variance components**, and the model (Equation 12-1) is called the **components of variance** or **random effects model.** To test hypotheses in this model, we require that the $\{\epsilon_{ij}\}$ are NID(0, σ^2), that the $\{\tau_i\}$ are NID(0, σ_τ^2), and that τ_i and ϵ_{ij} are independent.[1]

The sum of squares identity

$$SS_T = SS_{\text{Treatments}} + SS_E \tag{12-2}$$

is still valid. That is, we partition the total variability in the observations into a component that measures the variation between treatments ($SS_{\text{Treatments}}$) and a component that measures the variation within treatments (SS_E). Testing hypotheses about individual treatment effects is meaningless, so instead we test hypotheses about the variance component σ_τ^2:

$$\begin{aligned} H_0&: \sigma_\tau^2 = 0 \\ H_1&: \sigma_\tau^2 > 0 \end{aligned} \tag{12-3}$$

If $\sigma_\tau^2 = 0$, all treatments are identical; but if $\sigma_\tau^2 > 0$, variability exists between treatments. As before, SS_E/σ^2 is distributed as chi-square with $N - a$ degrees of freedom and, under the null hypothesis, $SS_{\text{Treatments}}/\sigma^2$ is distributed as chi-square with $a - 1$ degrees of freedom. Both random variables are independent. Thus, under the null hypothesis $\sigma_\tau^2 = 0$, the ratio

$$F_0 = \frac{\dfrac{SS_{\text{Treatments}}}{a-1}}{\dfrac{SS_E}{N-a}} = \frac{MS_{\text{Treatments}}}{MS_E} \tag{12-4}$$

is distributed as F with $a - 1$ and $N - a$ degrees of freedom. However, we need to examine the expected mean squares to fully describe the test procedure.

Consider

$$E(MS_{\text{Treatments}}) = \frac{1}{a-1} E(SS_{\text{Treatments}}) = \frac{1}{a-1} E\left[\sum_{i=1}^{a} \frac{y_{i.}^2}{n} - \frac{y_{..}^2}{N}\right]$$

$$= \frac{1}{a-1} E\left[\frac{1}{n}\sum_{i=1}^{a}\left(\sum_{j=1}^{n} \mu + \tau_i + \epsilon_{ij}\right)^2 - \frac{1}{N}\left(\sum_{i=1}^{a}\sum_{j=1}^{n} \mu + \tau_i + \epsilon_{ij}\right)^2\right]$$

When squaring and taking expectation of the quantities in brackets, we see that terms involving τ_i^2 are replaced by σ_τ^2 as $E(\tau_i) = 0$. Also, terms involving $\epsilon_{i.}^2$, $\epsilon_{..}^2$, and

[1] The assumption that the $\{\tau_i\}$ are independent random variables implies that the usual assumption of $\sum_{i=1}^{a} \tau_i = 0$ from the fixed effects model does not apply to the random effects model.

$\sum_{i=1}^{a}\sum_{j=1}^{n}\tau_i^2$ are replaced by $n\sigma^2$, $an\sigma^2$, and $an^2\sigma_\tau^2$, respectively. Furthermore, all cross-product terms involving τ_i and ϵ_{ij} have zero expectation. This leads to

$$E(MS_{\text{Treatments}}) = \frac{1}{a-1}[N\mu^2 + N\sigma_\tau^2 + a\sigma^2 - N\mu^2 - n\sigma_\tau^2 - \sigma^2]$$

or

$$E(MS_{\text{Treatments}}) = \sigma^2 + n\sigma_\tau^2 \tag{12-5}$$

Similarly, we may show that

$$E(MS_E) = \sigma^2 \tag{12-6}$$

From the expected mean squares, we see that under H_0 both the numerator and denominator of the test statistic (Equation 12-4) are unbiased estimators of σ^2, whereas under H_1 the expected value of the numerator is greater than the expected value of the denominator. Therefore, we should reject H_0 for values of F_0 that are too large. This implies an upper-tail, one-tail critical region, so we reject H_0 if $F_0 > F_{\alpha,a-1,N-a}$.

The computational procedure and analysis of the variance table for the random effects model are identical to those for the fixed effects case. The conclusions, however, are quite different because they apply to the entire population of treatments.

We are usually interested in estimating the variance components (σ^2 and σ_τ^2) in the model. The procedure that we use to estimate σ^2 and σ_τ^2 is called the **analysis of variance method** because it makes use of the lines in the analysis of variance table. The procedure consists of equating the expected mean squares to their observed values in the analysis of variance table and solving for the variance components. In equating observed and expected mean squares in the single-factor random effects model, we obtain

$$MS_{\text{Treatments}} = \sigma^2 + n\sigma_\tau^2$$

and

$$MS_E = \sigma^2$$

Therefore, the estimators of the variance components are

$$\hat{\sigma}^2 = MS_E \tag{12-7}$$

and

$$\hat{\sigma}_\tau^2 = \frac{MS_{\text{Treatments}} - MS_E}{n} \tag{12-8}$$

For unequal sample sizes, replace n in Equation 12-8 by

$$n_0 = \frac{1}{a-1}\left[\sum_{i=1}^{a} n_i - \frac{\sum_{i=1}^{a} n_i^2}{\sum_{i=1}^{a} n_i}\right] \tag{12-9}$$

The analysis of variance method of variance component estimation does not require the normality assumption. It does yield estimators of σ^2 and σ_τ^2 that are best quadratic unbiased (i.e., of all unbiased quadratic functions of the observations, these estimators have minimum variance).

Occasionally, the analysis of variance method produces a negative estimate of a variance component. Clearly, variance components are by definition nonnegative, so a negative estimate of a variance component is viewed with some concern. One course of action is to accept the estimate and use it as evidence that the true value of the variance component is zero, assuming that sampling variation led to the negative estimate. This has intuitive appeal, but it suffers from some theoretical difficulties. For instance, using zero in place of the negative estimate can disturb the statistical properties of other estimates. Another alternative is to reestimate the negative variance component using a method that always yields nonnegative estimates. Still another alternative is to consider the negative estimate as evidence that the assumed linear model is incorrect and reexamine the problem. Comprehensive treatment of variance component estimation is given by Searle (1971a, 1971b), Searle, Casella, and McCullogh (1992), and Burdick and Graybill (1990).

EXAMPLE 12-1

A textile company weaves a fabric on a large number of looms. It would like the looms to be homogeneous so that it obtains a fabric of uniform strength. The process engineer suspects that, in addition to the usual variation in strength within samples of fabric from the same loom, there may also be significant variations in strength between looms. To investigate this, she selects four looms at random and makes four strength determinations on the fabric manufactured on each loom. This experiment is run in random order, and the data obtained are shown in Table 12-1. The analysis of variance is conducted and is shown in Table 12-2 on the facing page. From the analysis of variance, we conclude that the looms in the plant differ significantly.

The variance components are estimated by $\hat{\sigma}^2 = 1.90$ and

$$\hat{\sigma}_\tau^2 = \frac{29.73 - 1.90}{4} = 6.96$$

Therefore, the variance of any observation on strength is estimated by

$$\hat{\sigma}_\tau = \hat{\sigma}^2 + \hat{\sigma}_\tau^2 = 1.90 + 6.96 = 8.86.$$

Most of this variability is attributable to differences *between* looms.

This example illustrates an important use of variance components—the isolating of different sources of variability that affect a product or system. The problem of product

Table 12-1 Strength Data for Example 12-1

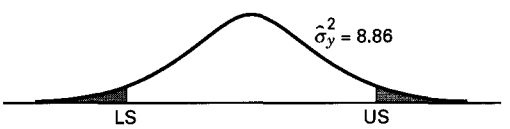
	Observations				
Looms	1	2	3	4	$y_{i.}$
1	98	97	99	96	390
2	91	90	93	92	366
3	96	95	97	95	383
4	95	96	99	98	388
					$1527 = y_{..}$

Table 12-2 Analysis of Variance for the Strength Data

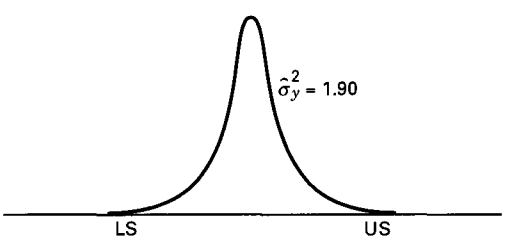
Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Looms	89.19	3	29.73	15.68	<0.001
Error	22.75	12	1.90		
Total	111.94	15			

variability frequently arises in quality assurance, and it is often difficult to isolate the sources of variability. For example, this study may have been motivated by too much variability in the strength of the fabric, as illustrated in Figure 12-1*a*. This graph displays the process output (fiber strength) modeled as a normal distribution with variance $\hat{\sigma}_y^2 = 8.86$. (This is the estimate of the variance of any observation on strength from Example 12-1.) Upper and lower specifications on strength are also shown in Figure 12-1*a*, and it is relatively easy to see that a fairly large proportion of the process output is outside the specifications (the shaded tail areas in Figure 12-1*a*). The process engineer has asked why so much fabric is defective and must be scrapped, reworked, or downgraded to a lower quality product. The answer is that most of the product strength variability is the result of differences between looms. Different loom performance could be the result of faulty setup, poor maintenance, ineffective supervision, poorly trained operators, defective input fiber, and so forth.

The process engineer must now try to isolate the specific causes of the difference in loom performance. If she could identify and eliminate these sources of between-loom variability, the variance of the process output could be reduced considerably, perhaps to as low as $\hat{\sigma}_y^2 = 1.90$, the estimate of the within-loom (error) variance component in Example 12-1. Figure 12-1*b* shows a normal distribution of fiber strength with $\hat{\sigma}_y^2 = 1.90$. Note that the proportion of defective product in the output has been dramatically reduced. Although it is unlikely that *all* of the between-loom variability can be eliminated, it is clear that a significant reduction in this variance component would greatly increase the quality of the fiber produced.



(*a*) Variability of process output.



(*b*) Variability of process output if $\sigma_\tau^2 = 0$.

Figure 12-1 Process output in the fiber strength problem.

We may easily find a confidence interval for the variance component σ^2. If the observations are normally and independently distributed, then $(N - a)MS_E/\sigma^2$ is distributed as χ^2_{N-a}. Thus,

$$P\left[\chi^2_{1-(\alpha/2),N-a} \leq \frac{(N-a)MS_E}{\sigma^2} \leq \chi^2_{\alpha/2,N-a}\right] = 1 - \alpha$$

and a $100(1 - \alpha)$ percent confidence interval for σ^2 is

$$\frac{(N-a)MS_E}{\chi^2_{\alpha/2,N-a}} \leq \sigma^2 \leq \frac{(N-a)MS_E}{\chi^2_{1-(\alpha/2),N-a}} \tag{12-10}$$

Now consider the variance component σ^2_τ. The point estimator of σ^2_τ is

$$\hat{\sigma}^2_\tau = \frac{MS_{\text{Treatments}} - MS_E}{n}$$

The random variable $(a - 1)MS_{\text{Treatments}}/(\sigma^2 + n\sigma^2_\tau)$ is distributed as χ^2_{a-1}, and $(N - a)MS_E/\sigma^2$ is distributed as χ^2_{N-a}. Thus, the probability distribution of $\hat{\sigma}^2_\tau$ is a linear combination of two chi-square random variables, say

$$u_1\chi^2_{a-1} - u_2\chi^2_{N-a}$$

where

$$u_1 = \frac{\sigma^2 + n\sigma^2_\tau}{n(a-1)} \quad \text{and} \quad u_2 = \frac{\sigma^2}{n(N-a)}$$

Unfortunately, a closed-form expression for the distribution of this linear combination of chi-square random variables cannot be obtained. Thus, an exact confidence interval for σ^2_τ cannot be constructed. Approximate procedures are given in Graybill (1961) and Searle (1971a). Also see Section 12-7.

It is easy to find an exact expression for a confidence interval on the ratio $\sigma^2_\tau/(\sigma^2_\tau + \sigma^2)$. This is a meaningful ratio because it reflects the *proportion* of the variance of an observation [recall that $V(y_{ij}) = \sigma^2_\tau + \sigma^2$] that is the result of differences between treatments. To develop this confidence interval for the case of a balanced design, note that $MS_{\text{Treatments}}$ and MS_E are independent random variables and, furthermore, that it can be shown that

$$\frac{MS_{\text{Treatments}}/(n\sigma^2_\tau + \sigma^2)}{MS_E/\sigma^2} \sim F_{a-1,N-a}$$

Thus,

$$\left(F_{1-\alpha/2,a-1,N-a} \leq \frac{MS_{\text{Treatments}}}{MS_E}\frac{\sigma^2}{n\sigma^2_\tau + \sigma^2} \leq F_{\alpha/2,a-1,N-a}\right) = 1 - \alpha \tag{12-11}$$

By rearranging Equation 12-11, we may obtain the following:

$$P\left(L \leq \frac{\sigma^2_\tau}{\sigma^2} \leq U\right) = 1 - \alpha \tag{12-12}$$

where

$$L = \frac{1}{n}\left(\frac{MS_{\text{Treatments}}}{MS_E}\frac{1}{F_{\alpha/2,a-1,N-a}} - 1\right) \tag{12-13a}$$

and

$$U = \frac{1}{n}\left(\frac{MS_{\text{Treatments}}}{MS_E}\frac{1}{F_{1-\alpha/2,a-1,N-a}} - 1\right) \tag{12-13b}$$

Note that L and U are $100(1-\alpha)$ percent lower and upper confidence limits, respectively, for the ratio σ_τ^2/σ^2. Therefore, a $100(1-\alpha)$ percent confidence interval for $\sigma_\tau^2/(\sigma_\tau^2+\sigma^2)$ is

$$\frac{L}{1+L} \leqslant \frac{\sigma_\tau^2}{\sigma_\tau^2+\sigma^2} \leqslant \frac{U}{1+U} \tag{12-14}$$

To illustrate this procedure, we find a 95 percent confidence interval on $\sigma_\tau^2/(\sigma_\tau^2+\sigma^2)$ for the strength data in Example 12-1. Recall that $MS_{\text{Treatments}} = 29.73$, $MS_E = 1.90$, $a = 4$, $n = 4$, $F_{0.025,3,12} = 4.47$, and $F_{0.975,3,12} = 1/F_{0.025,12,3} = 1/14.34 = 0.070$. Therefore, from Equation 12-13*a* and *b*,

$$L = \frac{1}{4}\left[\left(\frac{29.73}{1.90}\right)\left(\frac{1}{4.47}\right) - 1\right] = 0.625$$

$$U = \frac{1}{4}\left[\left(\frac{29.73}{1.90}\right)\left(\frac{1}{0.070}\right) - 1\right] = 54.883$$

and from Equation 12-12, the 95 percent confidence interval on $\sigma_\tau^2/(\sigma_\tau^2+\sigma^2)$ is

$$\frac{0.625}{1.625} \leqslant \frac{\sigma_\tau^2}{\sigma_\tau^2+\sigma^2} \leqslant \frac{54.883}{55.883}$$

or

$$0.39 \leqslant \frac{\sigma_\tau^2}{\sigma_\tau^2+\sigma^2} \leqslant 0.98$$

We conclude that variability between looms accounts for between 39 and 98 percent of the variance in the observed strength of the fabric produced. This confidence interval is relatively wide because of the small sample size that was used in the experiment. Clearly, however, the variability between looms (σ_τ^2) is not negligible.

12-2 THE TWO-FACTOR FACTORIAL WITH RANDOM FACTORS

Suppose that we have two factors, A and B, and that both factors have a large number of levels that are of interest (as in the previous section, we will assume that the number of levels is infinite). We will choose at random a levels of factor A and b levels of factor B and arrange these factor levels in a factorial experimental design. If the experiment is replicated n times, we may represent the observations by the linear model

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases} \tag{12-15}$$

where the model parameters τ_i, β_j, $(\tau\beta)_{ij}$, and ϵ_{ijk} are all independent random variables. We are also going to assume that the random variables τ_i, β_j, $(\tau\beta)_{ij}$, and ϵ_{ijk} are normally

distributed with mean zero and variances given by $V(\tau_i) = \sigma_\tau^2$, $V(\beta_j) = \sigma_\beta^2$, $V[(\tau\beta)_{ij}] = \sigma_{\tau\beta}^2$, and $V(\epsilon_{ijk}) = \sigma^2$. Therefore the variance of any observation is

$$V(y_{ijk}) = \sigma_\tau^2 + \sigma_\beta^2 + \sigma_{\tau\beta}^2 + \sigma^2 \tag{12-16}$$

and σ_τ^2, σ_β^2, $\sigma_{\tau\beta}^2$, and σ^2 are the **variance components**. The hypotheses that we are interested in testing are $H_0: \sigma_\tau^2 = 0$, $H_0: \sigma_\beta^2 = 0$, and $H_0: \sigma_{\tau\beta}^2 = 0$. Notice the similarity to the single-factor random effects model.

The numerical calculations in the analysis of variance remains unchanged; that is, SS_A, SS_B, SS_{AB}, SS_T, and SS_E are all calculated as in the fixed effects case. However, to form the test statistics, we must examine the **expected mean squares**. It may be shown that

$$\begin{aligned} E(MS_A) &= \sigma^2 + n\sigma_{\tau\beta}^2 + bn\sigma_\tau^2 \\ E(MS_B) &= \sigma^2 + n\sigma_{\tau\beta}^2 + an\sigma_\beta^2 \\ E(MS_{AB}) &= \sigma^2 + n\sigma_{\tau\beta}^2 \end{aligned} \tag{12-17}$$

and

$$E(MS_E) = \sigma^2$$

From the expected mean squares, we see that the appropriate statistic for testing the no-interaction hypothesis $H_0: \sigma_{\tau\beta}^2 = 0$ is

$$F_0 = \frac{MS_{AB}}{MS_E} \tag{12-18}$$

because under H_0 both numerator and denominator of F_0 have expectation σ^2, and only if H_0 is false is $E(MS_{AB})$ greater than $E(MS_E)$. The ratio F_0 is distributed as $F_{(a-1)(b-1),ab(n-1)}$. Similarly, for testing $H_0: \sigma_\tau^2 = 0$ we would use

$$F_0 = \frac{MS_A}{MS_{AB}} \tag{12-19}$$

which is distributed as $F_{a-1,(a-1)(b-1)}$, and for testing $H_0: \sigma_\beta^2 = 0$ the statistic is

$$F_0 = \frac{MS_B}{MS_{AB}} \tag{12-20}$$

which is distributed as $F_{b-1,(a-1)(b-1)}$. These are all upper-tail, one-tail tests. Notice that these test statistics are not the same as those used if both factors A and B are fixed. The expected mean squares are always used as a guide to test statistic construction.

In many experiments involving random factors, interest centers at least as much on estimating the variance components as on hypothesis testing. The variance components may be estimated by the **analysis of variance method**, that is, by equating the observed mean squares in the lines of the analysis of variance table to their expected values and solving for the variance components. This yields

$$\begin{aligned} \hat{\sigma}^2 &= MS_E \\ \hat{\sigma}_{\tau\beta}^2 &= \frac{MS_{AB} - MS_E}{n} \\ \hat{\sigma}_\beta^2 &= \frac{MS_B - MS_{AB}}{an} \\ \hat{\sigma}_\tau^2 &= \frac{MS_A - MS_{AB}}{bn} \end{aligned} \tag{12-21}$$

as the point estimates of the variance components in the two-factor random effects model. We will discuss other methods for obtaining point estimates of the variance components and procedures for constructing confidence intervals in Section 12-7.

EXAMPLE 12-2

A Measurement Systems Capability Study

Statistically designed experiments are frequently used to investigate the sources of variability that affect a system. A common industrial application is to use a designed experiment to study the components of variability in a measurement system. These studies are often called **gauge capability studies** or **gauge repeatability and reproducibility (R&R) studies**, because these are the components of variability that are of interest.

A typical gauge R&R experiment [from Montgomery (1996)] is shown in Table 12-3. An instrument or gauge is used to measure a critical dimension on a part. Twenty parts have been selected from the production process, and three randomly selected operators measure each part twice with this gauge. The order in which the measurements are made is completely randomized, so this is a two-factor factorial experiment with design factors parts and operators, with two replications. Both parts and operators are random factors. The variance component identity in Equation 12-15 applies; namely,

$$\sigma_y^2 = \sigma_\tau^2 + \sigma_\beta^2 + \sigma_{\tau\beta}^2 + \sigma^2$$

where σ_y^2 is the total variability (including variability due to the different parts, variability due to the different operators, and variability due to the gauge), σ_τ^2 is the variance component for parts, σ_β^2 is the variance component for operators, $\sigma_{\tau\beta}^2$ is the variance component that represents interaction between parts and operators, and σ^2 is the random

Table 12-3 The Measurement Systems Capability Experiment in Example 12-2

Part Number	Operator 1		Operator 2		Operator 3	
1	21	20	20	20	19	21
2	24	23	24	24	23	24
3	20	21	19	21	20	22
4	27	27	28	26	27	28
5	19	18	19	18	18	21
6	23	21	24	21	23	22
7	22	21	22	24	22	20
8	19	17	18	20	19	18
9	24	23	25	23	24	24
10	25	23	26	25	24	25
11	21	20	20	20	21	20
12	18	19	17	19	18	19
13	23	25	25	25	25	25
14	24	24	23	25	24	25
15	29	30	30	28	31	30
16	26	26	25	26	25	27
17	20	20	19	20	20	20
18	19	21	19	19	21	23
19	25	26	25	24	25	25
20	19	19	18	17	19	17

experimental error. Typically, the variance component σ^2 is called the gauge repeatability, because σ^2 can be thought of as reflecting the variation observed when the same part is measured by the same operator, and

$$\sigma_\beta^2 + \sigma_{\tau\beta}^2$$

is usually called the reproducibility of the gauge, because it reflects the additional variability in the measurement system resulting from use of the instrument by the operator. These experiments are usually performed with the objective of estimating the variance components.

Table 12-4 (on the facing page) shows the analysis of variance for this experiment. The computations were performed using the Balanced ANOVA routine in Minitab. Based on the P-values, we conclude that the effect of parts is large, operators may have a small effect, and that there is no significant part–operator interaction. We may use Equation 12-21 to estimate the variance components as follows:

$$\hat{\sigma}_\tau^2 = \frac{62.39 - 0.71}{(3)(2)} = 10.28$$

$$\hat{\sigma}_\beta^2 = \frac{1.31 - 0.71}{(20)(2)} = 0.015$$

$$\hat{\sigma}_{\tau\beta}^2 = \frac{0.71 - 0.99}{2} = -0.14$$

and

$$\hat{\sigma}^2 = 0.99$$

The bottom portion of the Minitab output in Table 12-4 contains the expected mean squares for the random model with numbers in parentheses representing the variance components [(4) represents σ^2, (3) represents $\sigma_{\tau\beta}^2$, etc.]. The estimates of the variance components are also given, along with the error term that was used in testing that variance component in the analysis of variance. We will discuss the terminology **unrestricted model** later; it has no relevance in random models.

Notice that the estimate of one of the variance components, $\hat{\sigma}_{\tau\beta}^2$, is negative. This is certainly not reasonable because by definition variances are nonnegative. Unfortunately, negative estimates of variance components can result when we use the analysis of variance method of estimation (this is considered one of its drawbacks). There are a variety of ways to deal with this. One possibility is to assume that the negative estimate means that the variance component is really zero and just set it to zero, leaving the other nonnegative estimates unchanged. Another approach is to estimate the variance components with a method that assures nonnegative estimates (we will discuss this briefly in Section 12-7). Finally, we could note that the P-value for the interaction term in Table 12-4 is very large, take this as evidence that $\sigma_{\tau\beta}^2$ really is zero, that there is no interaction effect, and fit a **reduced model** of the form

$$y_{ijk} = \mu + \tau_i + \beta_j + \epsilon_{ijk}$$

that does not include the interaction term. This is a relatively easy approach and one that often works nearly as well as more sophisticated methods.

Table 12-5 (page 522) shows the analysis of variance for the reduced model. Because

Table 12-4 Analysis of Variance (Minitab Balanced ANOVA) for Example 12-2

Analysis of Variance (Balanced Designs)

Factor	Type	Levels	Values						
part	random	20	1	2	3	4	5	6	7
			8	9	10	11	12	13	14
			15	16	17	18	19	20	
operator	random	3	1	2	3				

Analysis of Variance for y

Source	DF	SS	MS	F	P
part	19	1185.425	62.391	87.65	0.000
operator	2	2.617	1.308	1.84	0.173
part*operator	38	27.050	0.712	0.72	0.861
Error	60	59.500	0.992		
Total	119	1274.592			

Source	Variance component	Error term	Expected Mean Square for Each Term (using unrestricted model)
1 part	10.2798	3	(4) + 2(3) + 6(1)
2 operator	0.0149	3	(4) + 2(3) + 40(2)
3 part*operator	-0.1399	4	(4) + 2(3)
4 Error	0.9917		(4)

Table 12-5 Analysis of Variance for the Reduced Model, Example 12-2

Analysis of Variance (Balanced Designs)

```
Factor     Type Levels Values
part     random     20    1     2     3     4     5     6     7
                          8     9    10    11    12    13    14
                         15    16    17    18    19    20
operator random      3    1     2     3

Analysis of Variance for y

Source      DF         SS         MS       F       P
part        19  1185.425    62.391   70.64   0.000
operator     2     2.617     1.308    1.48   0.232
Error       98    86.550     0.883
Total      119  1274.592

Source          Variance  Error  Expected Mean Square for Each T
                component   term   (using unrestricted model)
 1 part           10.2513     3   (3) + 6(1)
 2 operator        0.0106     3   (3) + 40(2)
 3 Error           0.8832         (3)
```

there is no interaction term in the model, both main effects are tested against the error term, and the estimates of the variance components are

$$\hat{\sigma}_{\tau}^2 = \frac{62.39 - 0.88}{(3)(2)} = 10.25$$

$$\hat{\sigma}_{\beta}^2 = \frac{1.31 - 0.88}{(20)(2)} = 0.0108$$

$$\hat{\sigma}^2 = 0.88$$

Finally, we could estimate the variance of the gauge as the sum of the variance component estimates $\hat{\sigma}^2$ and $\hat{\sigma}_{\beta}^2$ as

$$\begin{aligned}\hat{\sigma}_{\text{gauge}}^2 &= \hat{\sigma}^2 + \hat{\sigma}_{\beta}^2 \\ &= 0.88 + 0.0108 \\ &= 0.8908\end{aligned}$$

The variability in the gauge appears small relative to the variability in the product. This is generally a desirable situation, implying that the gauge is capable of distinguishing among different grades of product.

12-3 THE TWO-FACTOR MIXED MODEL

We now consider the situation where one of the factors A is fixed and the other B is random. This is called the **mixed model** analysis of variance. The linear statistical model is

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases} \tag{12-22}$$

Here τ_i is a fixed effect, β_j is a random effect, the interaction $(\tau\beta)_{ij}$ is assumed to be a random effect, and ϵ_{ijk} is a random error. We also assume that the $\{\tau_i\}$ are fixed effects such that $\sum_{i=1}^{a}\tau_i = 0$ and β_j is a NID(0, σ_β^2) random variable. The interaction effect, $(\tau\beta)_{ij}$, is a normal random variable with mean 0 and variance $[(a-1)/a]\sigma_{\tau\beta}^2$; however, summing the interaction component over the fixed factor equals zero. That is,

$$\sum_{i=1}^{a}(\tau\beta)_{ij} = (\tau\beta)_{\cdot j} = 0 \qquad j = 1, 2, \ldots, b$$

This restriction implies that certain interaction elements at different levels of the fixed factor are not independent. In fact, we may show (see Problem 12-25) that

$$\text{Cov}[(\tau\beta)_{ij}, (\tau\beta)_{i'j}] = -\frac{1}{a}\sigma_{\tau\beta}^2 \qquad i \neq i'$$

The covariance between $(\tau\beta)_{ij}$ and $(\tau\beta)_{ij'}$ for $j \neq j'$ is zero, and the random error ϵ_{ijk} is NID(0, σ^2). Because the sum of the interaction effects over the levels of the fixed factor equals zero, this version of the mixed model is often called the **restricted model.**

In this model the variance of $(\tau\beta)_{ij}$ is defined as $[(a-1)/a]\sigma_{\tau\beta}^2$ rather than $\sigma_{\tau\beta}^2$ to simplify the expected mean squares. The assumption $(\tau\beta)_{\cdot j} = 0$ also has an effect on the expected mean squares, which we may show are

$$\begin{aligned} E(MS_A) &= \sigma^2 + n\sigma_{\tau\beta}^2 + \frac{bn\sum_{i=1}^{a}\tau_i^2}{a-1} \\ E(MS_B) &= \sigma^2 + an\sigma_\beta^2 \\ E(MS_{AB}) &= \sigma^2 + n\sigma_{\tau\beta}^2 \end{aligned} \tag{12-23}$$

and

$$E(MS_E) = \sigma^2$$

Therefore, the appropriate test statistic for testing that the means of the fixed factor effects are equal, or $H_0: \tau_i = 0$, is

$$F_0 = \frac{MS_A}{MS_{AB}}$$

for which the reference distribution is $F_{a-1,(a-1)(b-1)}$. For testing $H_0: \sigma_\beta^2 = 0$, the test statistic is

$$F_0 = \frac{MS_B}{MS_E}$$

with reference distribution $F_{b-1,ab(n-1)}$. Finally, for testing the interaction hypothesis $H_0: \sigma_{\tau\beta}^2 = 0$, we would use

$$F_0 = \frac{MS_{AB}}{MS_E}$$

which has reference distribution $F_{(a-1)(b-1),ab(n-1)}$.

In the mixed model, it is possible to estimate the fixed factor effects as

$$\begin{aligned} \hat{\mu} &= \bar{y}_{\cdots} \\ \hat{\tau}_i &= \bar{y}_{i\cdot\cdot} - \bar{y}_{\cdots} \qquad i = 1, 2, \ldots, a \end{aligned} \tag{12-24}$$

The variance components σ_β^2, $\sigma_{\tau\beta}^2$, and σ^2 may be estimated using the analysis of variance method. Eliminating the first equation from Equations 12-23 leaves three equations in three unknowns, whose solutions are

$$\hat{\sigma}_\beta^2 = \frac{MS_B - MS_E}{an}$$
$$\hat{\sigma}_{\tau\beta}^2 = \frac{MS_{AB} - MS_E}{n} \tag{12-25}$$

and

$$\hat{\sigma}^2 = MS_E$$

This general approach can be used to estimate the variance components in *any* mixed model. After eliminating the mean squares containing fixed factors, there will always be a set of equations remaining that can be solved for the variance components.

In mixed models the experimenter may be interested in testing hypotheses or constructing confidence intervals about individual treatment means for the fixed factor. In using such procedures, care must be exercised to use the proper standard error of the treatment mean. The standard error of the fixed effect treatment mean is

$$\left[\frac{\text{Mean square for testing the fixed effect}}{\text{Number of observations in each treatment mean}}\right]^{1/2} = \sqrt{\frac{MS_{AB}}{bn}}$$

Notice that this is just the standard error that we would use if this was a fixed effects model, except that MS_E has been replaced by the mean square used for hypothesis testing.

EXAMPLE 12-3

The Measurement Systems Capability Experiment Revisited

Reconsider the gauge R&R experiment described in Example 12-2. Suppose now that there are only three operators that use this gauge, so the operators are a fixed factor. However, because the parts are chosen at random, the experiment now involves a mixed model.

The analysis of variance for the mixed model is shown in Table 12-6 on the facing page. The computations were performed using the Balanced ANOVA routine in Minitab. We specified that the restricted model be used in the Minitab analysis. Minitab also generated the expected mean squares for this model. In the Minitab output, the quantity $Q[2]$ indicates a quadratic expression involving the fixed factor effect operator. That is, $Q[2] = \Sigma_{j=1}^{b}\beta_j^2/(b-1)$. The conclusions are similar to Example 12-2. The variance components may be estimated from Equation (12-25) as

$$\hat{\sigma}_{\text{Parts}}^2 = \frac{MS_{\text{Parts}} - MS_E}{an} = \frac{62.39 - 0.99}{(3)(2)} = 10.23$$
$$\hat{\sigma}_{\text{Parts}\times\text{operators}}^2 = \frac{MS_{\text{Parts}\times\text{operators}} - MS_E}{n} = \frac{0.71 - 0.99}{2} = -0.14$$
$$\hat{\sigma}^2 = MS_E = 0.99$$

These results are also given in the Minitab output. Once again, a negative estimate of the interaction variance component results. An appropriate course of action would be to

Table 12-6 Analysis of Variance (Minitab) for the Mixed Model in Example 12-3. The Restricted Model is Assumed.

Analysis of Variance (Balanced Designs)

Factor	Type	Levels	Values						
part	random	20	1	2	3	4	5	6	7
			8	9	10	11	12	13	14
			15	16	17	18	19	20	
operator	fixed	3	1	2	3				

Analysis of Variance for y

Source	DF	SS	MS	F	P
part	19	1185.425	62.391	62.92	0.000
operator	2	2.617	1.308	1.84	0.173
part*operator	38	27.050	0.712	0.72	0.861
Error	60	59.500	0.992		
Total	119	1274.592			

Source	Variance component	Error term	Expected Mean Square for Each Term (using restricted model)
1 part	10.2332	4	(4) + 6(1)
2 operator		3	(4) + 2(3) + 40Q[2]
3 part*operator	-0.1399	4	(4) + 2(3)
4 Error	0.9917		(4)

fit a reduced model, as we did in Example 12-2. In the case of a mixed model with two factors, this leads to the same results as in Example 12-2.

.....

Alternate Mixed Models

Several different versions of the mixed model have been proposed. These models differ from the restricted version of the mixed model discussed previously in the assumptions made about the random components. One of these alternate models is now briefly discussed.

Consider the model

$$y_{ijk} = \mu + \alpha_i + \gamma_j + (\alpha\gamma)_{ij} + \epsilon_{ijk}$$

where the α_i ($i = 1, 2, \ldots, a$) are fixed effects such that $\Sigma_{i=1}^{a}\alpha_i = 0$ and γ_j, $(\alpha\gamma)_{ij}$, and ϵ_{ijk} are uncorrelated random variables having zero means and variances $V(\gamma_j) = \sigma_\gamma^2$, $V[(\alpha\gamma)_{ij}] = \sigma_{\alpha\gamma}^2$, and $V(\epsilon_{ijk}) = \sigma^2$. Note that the restriction imposed previously on the interaction effect is not used here; consequently, this version of the mixed model is often called the **unrestricted mixed model**.

We can show that expected mean squares for this model are (refer to the supplemental text material for this chapter)

$$\begin{aligned} E(MS_A) &= \sigma^2 + n\sigma_{\alpha\gamma}^2 + \frac{bn\sum_{i=1}^{a}\alpha_i^2}{a-1} \\ E(MS_B) &= \sigma^2 + n\sigma_{\alpha\gamma}^2 + an\sigma_\gamma^2 \\ E(MS_{AB}) &= \sigma^2 + n\sigma_{\alpha\gamma}^2 \end{aligned} \tag{12-26}$$

and

$$E(MS_E) = \sigma^2$$

Comparing these expected mean squares with those in Equation 12-23, we note that the only obvious difference is the presence of the variance component $\sigma_{\alpha\gamma}^2$ in the expected mean square for the random effect. (Actually, there are other differences because of the different definitions of the variance of the interaction effect in the two models.) Consequently, we would test the hypothesis that the variance component for the random effect equals zero ($H_0: \sigma_\gamma^2 = 0$) using the statistic

$$F_0 = \frac{MS_B}{MS_{AB}}$$

as contrasted with testing $H_0: \sigma_\beta^2 = 0$ with $F_0 = MS_B/MS_E$ in the restricted model. The test should be more conservative using this model because MS_{AB} will generally be larger than MS_E.

The parameters in the two models are closely related. In fact, we may show that

$$\begin{aligned} \beta_j &= \gamma_j + (\overline{\alpha\gamma})_{.j} \\ (\tau\beta)_{ij} &= (\alpha\gamma)_{ij} + (\overline{\alpha\gamma})_{.j} \\ \sigma_\gamma^2 &= \sigma_\beta^2 + \frac{1}{a}\sigma_{\alpha\gamma}^2 \end{aligned}$$

and

$$\sigma_{\tau\beta}^2 = \sigma_{\alpha\gamma}^2$$

The analysis of variance method may be used to estimate the variance components. Referring to the expected mean squares, we find that the only change from Equations 12-25 is that

$$\hat{\sigma}^2_\gamma = \frac{MS_B - MS_{AB}}{an} \tag{12-27}$$

Both of these models are special cases of the mixed model proposed by Scheffé (1956a, 1959). This model assumes that the observations may be represented by

$$y_{ijk} = m_{ij} + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases}$$

where m_{ij} and ϵ_{ijk} are independent random variables. The structure of m_{ij} is

$$\begin{aligned} m_{ij} &= \mu + \tau_i + b_j + c_{ij} \\ E(m_{ij}) &= \mu + \tau_i \\ \sum_{i=1}^{a} \tau_i &= 0 \end{aligned}$$

and

$$c_{.j} = 0 \qquad j = 1, 2, \ldots, b$$

The variances and covariances of b_j and c_{ij} are expressed through the covariances of the m_{ij}. Furthermore, the random effects parameters in other formulations of the mixed model can be related to b_j and c_{ij}. The statistical analysis of Scheffé's model is identical to that for our restricted model, except that in general the statistic MS_A/MS_{AB} is not always distributed as F when $H_0: \tau_i = 0$ is true.

In light of this multiplicity of mixed models, a logical question is: Which model should one use? Most statisticians tend to prefer the restricted model, and it is the most widely encountered in the literature. The restricted model is actually slightly more general than the unrestricted model, because in the restricted model the covariance between two observations from the same level of the random factor can be either positive or negative, whereas this covariance can only be positive in the unrestricted model. If the correlative structure of the random components is not large, then either mixed model is appropriate, and there are only minor differences between these models. When we subsequently refer to mixed models, we assume the restricted model structure. However, if there are large correlations in the data, then Scheffé's model may have to be employed. The choice of model should always be dictated by the data. The article by Hocking (1973) is a clear summary of various mixed models.

EXAMPLE 12-4

The Unrestricted Model

Some computer software packages support only one mixed model. Minitab supports both the restricted and unrestricted model, although the default is to the unrestricted model. Table 12-7 (page 528) shows the Minitab output for the experiment in Example 12-3 using the unrestricted model. Note that the expected mean squares are in agreement with those in Equation 12-26. The conclusions are identical to those from the restricted model analysis, and the variance component estimates are very similar.

Table 12-7 Analysis of the Experiment in Example 12-3 Using the Unrestricted Model

Analysis of Variance (Balanced Designs)

Factor	Type	Levels	Values						
part	random	20	1	2	3	4	5	6	7
			8	9	10	11	12	13	14
			15	16	17	18	19	20	
operator	fixed	3	1	2	3				

Analysis of Variance for y

Source	DF	SS	MS	F	P
part	19	1185.425	62.391	87.65	0.000
operator	2	2.617	1.308	1.84	0.173
part*operator	38	27.050	0.712	0.72	0.861
Error	60	59.500	0.992		
Total	119	1274.592			

	Source	Variance component	Error term	Expected Mean Square for Each Term (using unrestricted model)
1	part	10.2798	3	(4) + 2(3) + 6(1)
2	operator		3	(4) + 2(3) + Q[2]
3	part*operator	-0.1399	4	(4) + 2(3)
4	Error	0.9917		(4)

12-4 SAMPLE SIZE DETERMINATION WITH RANDOM EFFECTS

The operating characteristic curves in the Appendix may be used for sample size determination in experiments with random factors. We begin with the single-factor random effects model of Section 12-1. The type II error probability for the random effects model is

$$\begin{aligned}\beta &= 1 - P\{\text{Reject } H_0 | H_0 \text{ is false}\} \\ &= 1 - P\{F_0 > F_{\alpha,a-1,N-a} | \sigma_\tau^2 > 0\}\end{aligned} \tag{12-28}$$

Once again, the distribution of the test statistic $F_0 = MS_{\text{Treatments}}/MS_E$ under the alternative hypothesis is needed. It can be shown that if H_1 is true ($\sigma_\tau^2 > 0$), the distribution of F_0 is central F with $a - 1$ and $N - a$ degrees of freedom.

Because the type II error probability of the random effects model is based on the usual central F distribution, we could use the tables of the F distribution in the Appendix to evaluate Equation 12-28. However, it is simpler to determine the sensitivity of the test through the use of operating characteristic curves. A set of these curves for various values of numerator degrees of freedom, denominator degrees of freedom, and α of 0.05 or 0.01 is provided in Chart VI of the Appendix. These curves plot the probability of type II error against the parameter λ, where

$$\lambda = \sqrt{1 + \frac{n\sigma_\tau^2}{\sigma^2}} \tag{12-29}$$

Note that λ involves two unknown parameters, σ^2 and σ_τ^2. We may be able to estimate σ_τ^2 if we have an idea about how much variability in the population of treatments it is important to detect. An estimate of σ^2 may be chosen using prior experience or judgment. Sometimes it is helpful to define the value of σ_τ^2 we are interested in detecting in terms of the ratio σ_τ^2/σ^2.

EXAMPLE 12-5

Suppose we have five treatments selected at random with six observations per treatment and $\alpha = 0.05$, and we wish to determine the power of the test if σ_τ^2 is equal to σ^2. Because $a = 5$, $n = 6$, and $\sigma_\tau^2 = \sigma^2$, we may compute

$$\lambda = \sqrt{1 + 6(1)} = 2.646$$

From the operating characteristic curve with $a - 1 = 4, N - a = 25$ degrees of freedom, and $\alpha = 0.05$, we find that

$$\beta \simeq 0.20$$

and thus the power is approximately 0.80.

We can also use the percentage increase in the standard deviation of an observation method to determine sample size. If the treatments are homogeneous, then the standard deviation of an observation selected at random is σ. However, if the treatments are different, the standard deviation of a randomly chosen observation is

$$\sqrt{\sigma^2 + \sigma_\tau^2}$$

If P is the fixed percentage increase in the standard deviation of an observation beyond which rejection of the null hypothesis is desired,

$$\frac{\sqrt{\sigma^2 + \sigma_\tau^2}}{\sigma} = 1 + 0.01P$$

or

$$\frac{\sigma_\tau^2}{\sigma^2} = (1 + 0.01P)^2 - 1$$

Therefore, using Equation 12-29, we find that

$$\lambda = \sqrt{1 + \frac{n\sigma_\tau^2}{\sigma^2}} = \sqrt{1 + n[(1 + 0.01P)^2 - 1]} \tag{12-30}$$

For a given P, the operating characteristic curves in Appendix Chart VI can be used to find the desired sample size.

We can also use the operating characteristic curves for sample size determination for the two-factor random effects model and the mixed model. Appendix Chart VI is used for the random effects model. The parameter λ, numerator degrees of freedom, and denominator degrees of freedom are shown in the top half of Table 12-8. For the mixed model, both Charts V and VI in the Appendix must be used. The appropriate values for Φ^2 and λ are shown in the bottom half of Table 12-8.

Table 12-8 Operating Characteristic Curve Parameters for Tables V and VI of the Appendix for the Two-Factor Random Effects and Mixed Models

The Random Effects Model

Factor	λ	Numerator Degrees of Freedom	Denominator Degrees of Freedom
A	$\sqrt{1 + \frac{bn\sigma_\tau^2}{\sigma^2 + n\sigma_{\tau\beta}^2}}$	$a - 1$	$(a - 1)(b - 1)$
B	$\sqrt{1 + \frac{an\sigma_\beta^2}{\sigma^2 + n\sigma_{\tau\beta}^2}}$	$b - 1$	$(a - 1)(b - 1)$
AB	$\sqrt{1 + \frac{n\sigma_{\tau\beta}^2}{\sigma^2}}$	$(a - 1)(b - 1)$	$ab(n - 1)$

The Mixed Model

Factor	Parameter	Numerator Degrees of Freedom	Denominator Degrees of Freedom	Appendix Chart
A (Fixed)	$\Phi^2 = \frac{bn\sum_{i=1}^{a}\tau_i^2}{a[\sigma^2 + n\sigma_{\tau\beta}^2]}$	$a - 1$	$(a - 1)(b - 1)$	V
B (Random)	$\lambda = \sqrt{1 + \frac{an\sigma_\beta^2}{\sigma^2}}$	$b - 1$	$ab(n - 1)$	VI
AB	$\lambda = \sqrt{1 + \frac{n\sigma_{\tau\beta}^2}{\sigma^2}}$	$(a - 1)(b - 1)$	$ab(n - 1)$	VI

12-5 RULES FOR EXPECTED MEAN SQUARES

An important part of any experimental design problem is conducting the analysis of variance. This involves determining the sum of squares for each component in the model and the number of degrees of freedom associated with each sum of squares. Then, to construct appropriate test statistics, the expected mean squares must be determined. In complex design situations, particularly those involving random or mixed models, it is frequently helpful to have a formal procedure for this process.

We will present a set of rules for writing down the expected mean squares for any balanced factorial, nested,[2] or nested factorial experiment. (Note that partially balanced arrangements, such as Latin squares and incomplete block designs, are specifically excluded.) These rules are discussed by several authors, including Scheffé (1959), Bennett and Franklin (1954), Cornfield and Tukey (1956), and Searle (1971a, 1971b). By examining the expected mean squares, one may develop the appropriate statistic for testing hypotheses about any model parameter. The test statistic is a ratio of mean squares that is chosen such that the expected value of the **numerator** mean square differs from the expected value of the **denominator** mean square only by the variance component or the fixed factor in which we are interested.

It is always possible to determine the expected mean squares in any model as we did in Chapter 3, that is, by the direct application of the expectation operator. This **brute force** method, as it is often called, can be very tedious. The rules that follow always produce the expected mean squares without resorting to the brute force approach, and, with practice, they become relatively simple to use. When applied to a mixed model, these rules produce expected mean squares that are consistent with the assumptions for the **restricted mixed model** of Section 12-3. We illustrate the rules using the two-factor fixed effects factorial model.

Rule 1. The error term in the model, $\epsilon_{ij\ldots m}$, is written as $\epsilon_{(ij\ldots)m}$, where the subscript m denotes the replication subscript. For the two-factor model, this rule implies that ϵ_{ijk} becomes $\epsilon_{(ij)k}$.

Rule 2. In addition to an overall mean (μ) and an error term [$\epsilon_{(ij\ldots)m}$], the model contains all the main effects and any interactions that the experimenter assumes exist. If all possible interactions between k factors exist, then there are $\binom{k}{2}$ two-factor interactions, $\binom{k}{3}$ three-factor interactions, . . . , 1 k-factor interaction. If one of the factors in a term appears in parentheses, then there is no interaction between that factor and the other factors in that term.

Rule 3. For each term in the model, divide the subscripts into three classes: (a) live—those subscripts that are present in the term and are not in parentheses; (b) dead—those subscripts that are present in the term and are in parentheses; and (c) absent—those subscripts that are present in the model but not in that particular term.

Thus, in $(\tau\beta)_{ij}$, i and j are live and k is absent, and in $\epsilon_{(ij)k}$, k is live and i and j are dead.

[2] Nested designs are discussed in Chapter 13.

Rule 4. Degrees of freedom. The number of degrees of freedom for any term in the model is the product of the number of levels associated with each dead subscript and the number of levels minus 1 associated with each live subscript.

For example, the number of degrees of freedom associated with $(\tau\beta)_{ij}$ is $(a - 1)(b - 1)$, and the number of degrees of freedom associated with $\epsilon_{(ij)k}$ is $ab(n - 1)$.

Rule 5. Each term in the model has either a variance component (random effect) or a fixed factor (fixed effect) associated with it. If an interaction contains at least one random effect, the entire interaction is considered as random. A variance component has Greek letters as subscripts to identify the particular random effect. Thus, in a two-factor mixed model with factor A fixed and factor B random, the variance component for B is σ_β^2, and the variance component for AB is $\sigma_{\tau\beta}^2$. A fixed effect is always represented by the sum of squares of the model components associated with that factor divided by its degrees of freedom. In our example, the effect of A is

$$\frac{\sum_{i=1}^{a} \tau_i^2}{a - 1}$$

Rule 6. Expected mean squares. To obtain the expected mean squares, prepare the following table. There is a row for each model component (mean square) and a column for each subscript. Over each subscript, write the number of levels of the factor associated with that subscript and whether the factor is fixed (F) or random (R). Replicates are always considered to be random.

(a) In each row, write 1 if one of the dead subscripts in the row component matches the subscript in the column:

	F	F	R
	a	b	n
Factor	i	j	k
τ_i			
β_j			
$(\tau\beta)_{ij}$			
$\epsilon_{(ij)k}$	1	1	

(b) In each row, if any of the subscripts on the row component match the subscript in the column, write 0 if the column is headed by a fixed factor and 1 if the column is headed by a random factor:

	F	F	R
	a	b	n
Factor	i	j	k
τ_i	0		
β_j		0	
$(\tau\beta)_{ij}$	0	0	
$\epsilon_{(ij)k}$	1	1	1

(c) In the remaining empty row positions, write the number of levels shown above the column heading:

Factor	F a i	F b j	R n k
τ_i	0	b	n
β_j	a	0	n
$(\tau\beta)_{ij}$	0	0	n
$\epsilon_{(ij)k}$	1	1	1

(d) To obtain the expected mean square for any model component, first cover all columns headed by live subscripts on that component. Then, in each row that contains *at least* the *same* subscripts as those on the component being considered, take the product of the visible numbers and multiply by the appropriate fixed or random factor from rule 1. The sum of these quantities is the expected mean square of the model component being considered. To find $E(MS_A)$, for example, cover column i. The product of the visible numbers in the rows that contain at least subscript i are bn (row 1), 0 (row 3), and 1 (row 4). Note that i is missing in row 2. Therefore, the expected mean square is

$$E(MS_A) = \sigma^2 + \frac{bn \sum_{i=1}^{a} \tau_i^2}{a - 1}$$

The complete table of expected mean squares for this design is shown in Table 12-9. Tables 12-10 and 12-11 (page 534) display the expected mean square derivations for the two-factor random and mixed models, respectively. Notice that the restricted version of the mixed model has been assumed in producing the expected mean squares. A three-factor factorial design is treated in the following example.

EXAMPLE 12-6

Consider a three-factor factorial experiment with a levels of factor A, b levels of factor B, c levels of factor C, and n replicates. The analysis of this design, assuming that all the factors are fixed effects, is given in Section 5-4. We now determine the expected

Table 12-9 Expected Mean Square Derivation, Two-Factor Fixed Effects Model

Factor	F a i	F b j	R n k	Expected Mean Square
τ_i	0	b	n	$\sigma^2 + \frac{bn\Sigma\tau_i^2}{a - 1}$
β_j	a	0	n	$\sigma^2 + \frac{an\Sigma\beta_j^2}{b - 1}$
$(\tau\beta)_{ij}$	0	0	n	$\sigma^2 + \frac{n\Sigma\Sigma(\tau\beta)_{ij}^2}{(a - 1)(b - 1)}$
$\epsilon_{(ij)k}$	1	1	1	σ^2

Table 12-10 Expected Mean Square Derivation, Two-Factor Random Effects Model

Factor	R a i	R b j	R n k	Expected Mean Square
τ_i	1	b	n	$\sigma^2 + n\sigma^2_{\tau\beta} + bn\sigma^2_{\tau}$
β_j	a	1	n	$\sigma^2 + n\sigma^2_{\tau\beta} + an\sigma^2_{\beta}$
$(\tau\beta)_{ij}$	1	1	n	$\sigma^2 + n\sigma^2_{\tau\beta}$
$\epsilon_{(ij)k}$	1	1	1	σ^2

Table 12-11 Expected Mean Square Derivation, Two-Factor Mixed Model

Factor	F a i	R b j	R n k	Expected Mean Square
τ_i	0	b	n	$\sigma^2 + n\sigma^2_{\tau\beta} + \dfrac{bn\Sigma\tau_i^2}{a-1}$
β_j	a	1	n	$\sigma^2 + an\sigma^2_{\beta}$
$(\tau\beta)_{ij}$	0	1	n	$\sigma^2 + n\sigma^2_{\tau\beta}$
$\epsilon_{(ij)k}$	1	1	1	σ^2

Table 12-12 Expected Mean Square Derivation, Three-Factor Random Effects Model

Factor	R a i	R b j	R c k	R n l	Expected Mean Squares
τ_i	1	b	c	n	$\sigma^2 + cn\sigma^2_{\tau\beta} + bn\sigma^2_{\tau\gamma} + n\sigma^2_{\tau\beta\gamma} + bcn\sigma^2_{\tau}$
β_j	a	1	c	n	$\sigma^2 + cn\sigma^2_{\tau\beta} + an\sigma^2_{\beta\gamma} + n\sigma^2_{\tau\beta\gamma} + acn\sigma^2_{\beta}$
γ_k	a	b	1	n	$\sigma^2 + bn\sigma^2_{\tau\gamma} + an\sigma^2_{\beta\gamma} + n\sigma^2_{\tau\beta\gamma} + abn\sigma^2_{\gamma}$
$(\tau\beta)_{ij}$	1	1	c	n	$\sigma^2 + n\sigma^2_{\tau\beta\gamma} + cn\sigma^2_{\tau\beta}$
$(\tau\gamma)_{ik}$	1	b	1	n	$\sigma^2 + n\sigma^2_{\tau\beta\gamma} + bn\sigma^2_{\tau\gamma}$
$(\beta\gamma)_{jk}$	a	1	1	n	$\sigma^2 + n\sigma^2_{\tau\beta\gamma} + an\sigma^2_{\beta\gamma}$
$(\tau\beta\gamma)_{ijk}$	1	1	1	n	$\sigma^2 + n\sigma^2_{\tau\beta\gamma}$
ϵ_{ijkl}	1	1	1	1	σ^2

mean squares assuming that all the factors are *random*. The appropriate statistical model is

$$y_{ijkl} = \mu + \tau_i + \beta_j + \gamma_k + (\tau\beta)_{ij} + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} + (\tau\beta\gamma)_{ijk} + \epsilon_{ijkl}$$

Using the rules previously described, the expected mean squares are derived in Table 12-12 on the facing page.

We notice, by examining the expected mean squares in Table 12-12, that if A, B, and C are all random factors, then no exact test exists for the main effects. That is, if we wish to test the hypothesis $\sigma_\tau^2 = 0$, we cannot form a ratio of two expected mean squares such that the only term in the numerator that is not in the denominator is $bcn\sigma_\tau^2$. The same phenomenon occurs for the main effects of B and C. Notice that proper tests do exist for the two- and three-factor interactions. However, it is likely that tests on the main effects are of central importance to the experimenter. Therefore, how should the main effects be tested? This problem is considered in the next section.

12-6 APPROXIMATE *F* TESTS

In factorial experiments with three or more factors involving a random or mixed model and certain other, more complex designs, there are frequently no exact test statistics for certain effects in the models. One possible solution to this dilemma is to assume that certain interactions are negligible. To illustrate, if we could reasonably assume that all the two-factor interactions in Example 12-6 are negligible, then we could put $\sigma_{\tau\beta}^2 = \sigma_{\tau\gamma}^2 = \sigma_{\beta\gamma}^2 = 0$, and tests for main effects could be conducted.

Although this seems to be an attractive possibility, we must point out that there must be something in the nature of the process—or some strong prior knowledge—for us to assume that one or more of the interactions are negligible. In general, this assumption is not easily made, nor should it be taken lightly. We should not eliminate certain interactions from the model without conclusive evidence that it is appropriate to do so. A procedure advocated by some experimenters is to test the interactions first, then set at zero those interactions found to be insignificant, and then assume that these interactions are zero when testing other effects in the same experiment. Although sometimes done in practice, this procedure can be dangerous because any decision regarding an interaction is subject to both type I and type II errors.

A variation of this idea is to **pool** certain mean squares in the analysis of variance to obtain an estimate of error with more degrees of freedom. For instance, suppose that in Example 12-6 the test statistic $F_0 = MS_{ABC}/MS_E$ was not significant. Thus, $H_0: \sigma_{\tau\beta\gamma}^2 = 0$ is not rejected, and *both* MS_{ABC} and MS_E estimate the error variance σ^2. The experimenter might consider pooling or combining MS_{ABC} and MS_E according to

$$MS_{E'} = \frac{abc(n-1)MS_E + (a-1)(b-1)(c-1)MS_{ABC}}{abc(n-1) + (a-1)(b-1)(c-1)}$$

so that $E(MS_{E'}) = \sigma^2$. Note that $MS_{E'}$ has $abc(n-1) + (a-1)(b-1)(c-1)$ degrees of freedom, compared to $abc(n-1)$ degrees of freedom for the original MS_E.

The danger of pooling is that one may make a type II error and combine the mean square for a factor that really *is* significant with error, thus obtaining a new residual mean

square ($MS_{E'}$) that is too large. This will make other significant effects more difficult to detect. On the other hand, if the original error mean square has a very small number of degrees of freedom (e.g., less than six), the experimenter may have much to gain by pooling because it could potentially increase the precision of further tests considerably. A reasonably practical procedure is as follows. If the original error mean square has six or more degrees of freedom, do not pool. If the original error mean square has fewer than six degrees of freedom, pool only if the F statistic for the mean square to be pooled is not significant at a large value of α, such as $\alpha = 0.25$.

If we cannot assume that certain interactions are negligible and we still need to make inferences about those effects for which exact tests do not exist, a procedure attributed to Satterthwaite (1946) can be employed. Satterthwaite's method uses **linear combinations of mean squares**, for example,

$$MS' = MS_r + \cdots + MS_s \tag{12-31}$$

and

$$MS'' = MS_u + \cdots + MS_v \tag{12-32}$$

where the mean squares in Equations 12-31 and 12-32 are chosen so that $E(MS') - E(MS'')$ is equal to a multiple of the effect (the model parameter or variance component) considered in the null hypothesis. Then the test statistic would be

$$F = \frac{MS'}{MS''} \tag{12-33}$$

which is distributed approximately as $F_{p,q}$, where

$$p = \frac{(MS_r + \cdots + MS_s)^2}{MS_r^2/f_r + \cdots + MS_s^2/f_s} \tag{12-34}$$

and

$$q = \frac{(MS_u + \cdots + MS_v)^2}{MS_u^2/f_u + \cdots + MS_v^2/f_v} \tag{12-35}$$

In p and q, f_i is the number of degrees of freedom associated with the mean square MS_i. There is no assurance that p and q will be integers, so it may be necessary to interpolate in the tables of the F distribution. For example, in the three-factor random effects model (Table 12-12), it is relatively easy to see that an appropriate test statistic for $H_0: \sigma_\tau^2 = 0$ would be $F = MS'/MS''$, with

$$MS' = MS_A + MS_{ABC}$$

and

$$MS'' = MS_{AB} + MS_{AC}$$

The degrees of freedom for F would be computed from Equations 12-34 and 12-35.

The theory underlying this test is that both the numerator and the denominator of the test statistic (Equation 12-33) are distributed approximately as multiples of chi-square

random variables, and because no mean square appears in both the numerator or denominator of Equation 12-33, the numerator and denominator are independent. Thus F in Equation 12-33 is distributed approximately as $F_{p,q}$. Satterthwaite remarks that caution should be used in applying the procedure when some of the mean squares in MS' and MS'' are involved negatively. Gaylor and Hopper (1969) report that if $MS' = MS_1 - MS_2$, then Satterthwaite's approximation holds reasonably well if

$$\frac{MS_1}{MS_2} > F_{0.025,f_2,f_1} \times F_{0.50,f_2,f_2}$$

and if $f_1 \leq 100$ and $f_2 \geq f_1/2$.

EXAMPLE 12-7

The pressure drop measured across an expansion value in a turbine is being studied. The design engineer considers the important variables that influence pressure drop reading to be gas temperature on the inlet side (A), operator (B), and the specific pressure gauge used by the operator (C). These three factors are arranged in a factorial design, with gas temperature fixed, and operator and pressure gauge random. The coded data for two replicates are shown in Table 12-13. The linear model for this design is

$$y_{ijkl} = \mu + \tau_i + \beta_j + \gamma_k + (\tau\beta)_{ij} + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} + (\tau\beta\gamma)_{ijk} + \epsilon_{ijkl}$$

where τ_i is the effect of the gas temperature (A), β_j is the operator effect (B), and γ_k is the effect of the pressure gauge (C).

The analysis of variance is shown in Table 12-14. A column entitled "Expected Mean Squares" has been added to this table, and the entries in this column are derived by the methods discussed in Section 12-5. From the Expected Mean Squares column, we observe that exact tests exist for all effects except the main effect A. Results for these tests are shown in Table 12-14 on the facing page. To test the gas temperature effect, or $H_0: \tau_i = 0$, we could use the statistic

$$F = \frac{MS'}{MS''}$$

Table 12-13 Coded Pressure Drop Data for the Turbine Experiment

Pressure Gauge (C)	Gas Temperature (A)											
	60°F				75°F				90°F			
	Operator (B)				Operator (B)				Operator (B)			
	1	2	3	4	1	2	3	4	1	2	3	4
1	−2	0	−1	4	14	6	1	−7	−8	−2	−1	−2
	−3	−9	−8	4	14	0	2	6	−8	20	−2	1
2	−6	−5	−8	−3	22	8	6	−5	−8	1	−9	−8
	4	−1	−2	−7	24	6	2	2	3	−7	−8	3
3	−1	−4	0	−2	20	2	3	−5	−2	−1	−4	1
	−2	−8	−7	4	16	0	0	−1	−1	−2	−7	3

Table 12-14 Analysis of Variance for the Pressure Drop Data

Source of Variation	Sum of Squares	Degrees of Freedom	Expected Mean Squares	Mean Square	F_0	P-Value
Temperature, A	1023.36	2	$\sigma^2 + bn\sigma^2_{\tau\gamma} + cn\sigma^2_{\tau\beta} + n\sigma^2_{\tau\beta\gamma} + \frac{bcn\Sigma\tau_i^2}{a-1}$	511.68	2.22	0.17
Operator, B	423.82	3	$\sigma^2 + an\sigma^2_{\beta\gamma} + acn\sigma^2_{\beta}$	141.27	4.05	0.07
Pressure gauge, C	7.19	2	$\sigma^2 + an\sigma^2_{\beta\gamma} + abn\sigma^2_{\gamma}$	3.60	0.10	0.90
AB	1211.97	6	$\sigma^2 + n\sigma^2_{\tau\beta\gamma} + cn\sigma^2_{\tau\beta}$	202.00	14.59	<0.01
AC	137.89	4	$\sigma^2 + n\sigma^2_{\tau\beta\gamma} + bn\sigma^2_{\tau\gamma}$	34.47	2.49	0.10
BC	209.47	6	$\sigma^2 + an\sigma^2_{\beta\gamma}$	34.91	1.63	0.17
ABC	166.11	12	$\sigma^2 + n\sigma^2_{\tau\beta\gamma}$	13.84	0.65	0.79
Error	770.50	36	σ^2	21.40		
Total	3950.32	71				

where

$$MS' = MS_A + MS_{ABC}$$

and

$$MS'' = MS_{AB} + MS_{AC}$$

because

$$E(MS') - E(MS'') = \frac{bcn\Sigma\tau_i^2}{a-1}$$

To determine the test statistic for $H_0: \tau_i = 0$, we compute

$$\begin{aligned} MS' &= MS_A + MS_{ABC} \\ &= 511.68 + 13.84 = 525.52 \\ MS'' &= MS_{AB} + MS_{AC} \\ &= 202.00 + 34.47 = 236.47 \end{aligned}$$

and

$$F = \frac{MS'}{MS''} = \frac{525.52}{236.47} = 2.22$$

The degrees of freedom for this statistic are found from Equations 12-34 and 12-35 as follows:

$$\begin{aligned} p &= \frac{(MS_A + MS_{ABC})^2}{MS_A^2/2 + MS_{ABC}^2/12} \\ &= \frac{(525.52)^2}{(511.68)^2/2 + (13.84)^2/12} = 2.11 \simeq 2 \end{aligned}$$

and

$$\begin{aligned} q &= \frac{(MS_{AB} + MS_{AC})^2}{MS_{AB}^2/6 + MS_{AC}^2/4} \\ &= \frac{(236.47)^2}{(202.00)^2/6 + (34.47)^2/4} = 7.88 \simeq 8 \end{aligned}$$

Comparing $F = 2.22$ to $F_{0.05,2,8} = 4.46$, we cannot reject H_0. The P-value is approximately $P = 0.17$.

The AB, or temperature–operator, interaction is large, and there is some indication of an AC, or temperature–gauge, interaction. The graphical analysis of the AB and AC interactions, shown in Figure 12-2 (page 540), indicates that the effect of temperature may be large when operator 1 and gauge 3 are used. Thus, it seems possible that the main effects of temperature and operator are masked by the large AB interaction.

Table 12-15 (page 541) presents the Minitab Balanced ANOVA output for the experiment in Example 12-7. We have specified the **restricted model**. $Q[1]$ represents the fixed effect of gas pressure. Notice that the entries in the analysis of variance table are

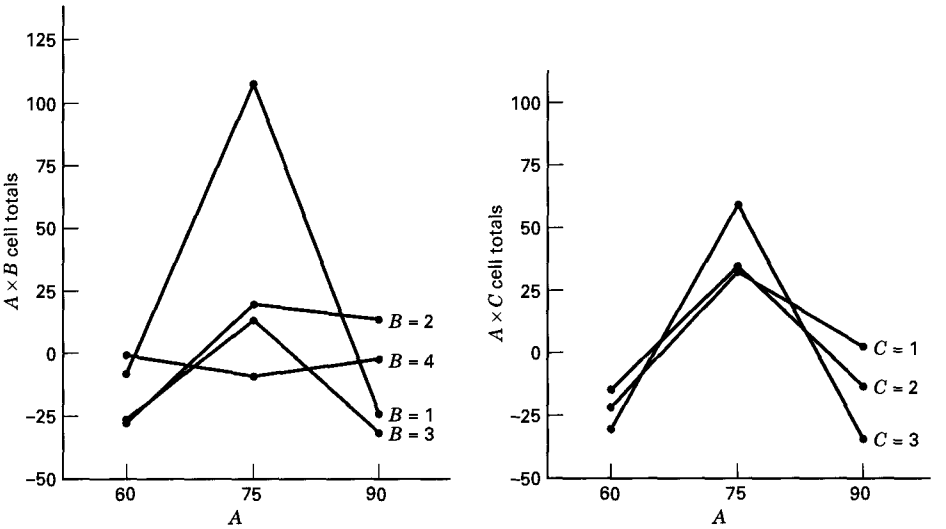


Figure 12-2 Interactions in pressure drop experiment.

in general agreement with those in Table 12-14, except for the F test on gas temperature (factor A). Minitab notes that the test is not an exact test (which we see from the expected mean squares). The Synthesized Test constructed by Minitab is actually Satterthwaite's procedure, but it uses a different test statistic than we did. Note that, from the Minitab output, the error mean square for testing factor A is

$$(4) + (5) - (7) = MS_{AB} + MS_{AC} - MS_{ABC}$$

for which the expected value is

$$\begin{aligned} E[(4) + (5) - (7)] &= \sigma^2 + n\sigma^2_{\tau\beta\gamma} + cn\sigma^2_{\tau\beta} + \sigma^2 + n\sigma^2_{\tau\beta\gamma} \\ &\quad + bn\sigma^2_{\tau\gamma} - (\sigma^2 + n\sigma^2_{\tau\beta\gamma}) \\ &= \sigma^2 + n\sigma^2_{\tau\beta\gamma} + cn\sigma^2_{\tau\beta} + bn\sigma^2_{\tau\gamma} \end{aligned}$$

which is an appropriate error mean square for testing the mean effect of A. This nicely illustrates that there can be more than one way to construct the synthetic mean squares used in Satterthwaite's procedure. However, we would generally prefer the linear combination of mean squares we selected instead of the one chosen by Minitab because it does not have any mean squares involved negatively in the linear combinations.

The analysis of Example 12-7, assuming the unrestricted model, is presented in Table 12-16 (page 542). The principal difference from the restricted model is that now the expected values of the mean squares for all three mean effects are such that no exact test exists. In the restricted model, the two random mean effects could be tested against their interaction, but now the expected mean square for B involves $\sigma^2_{\tau\beta\gamma}$ and $\sigma^2_{\tau\beta}$, and the expected mean square for C involves $\sigma^2_{\tau\beta\gamma}$ and $\sigma^2_{\tau\gamma}$. Once again, Minitab constructs synthetic mean squares and tests these effects with Satterthwaite's procedure. The overall conclusions are not radically different from the restricted model analysis, other than the large change in the estimate of the operator variance component. The unrestricted model produces a negative estimate of σ^2_{β}. Because the gauge factor is not significant in either analysis, it is possible that some model reduction is in order.

Factor	Type	Levels	Values			
GasT	fixed	3	60	75	90	
Operator	random	4	1	2	3	4
Gauge	random	3	1	2	3	

Analysis of Variance for Drop

Source	DF	SS	MS	F	P	
GasT	2	1023.36	511.68	2.30	0.171	x
Operator	3	423.82	141.27	4.05	0.069	
Gauge	2	7.19	3.60	0.10	0.904	
GasT*Operator	6	1211.97	202.00	14.59	0.000	
GasT*Gauge	4	137.89	34.47	2.49	0.099	
Operator*Gauge	6	209.47	34.91	1.63	0.167	
GasT*Operator*Gauge	12	166.11	13.84	0.65	0.788	
Error	36	770.50	21.40			
Total	71	3950.32				

x Not an exact F-test.

Source	Variance component	Error term	Expected Mean Square for Each Term (using restricted model)
1 GasT		*	(8) + 2(7) + 8(5) + 6(4) + 24Q[1]
2 Operator	5.909	6	(8) + 6(6) + 18(2)
3 Gauge	-1.305	6	(8) + 6(6) + 24(3)
4 GasT*Operator	31.359	7	(8) + 2(7) + 6(4)
5 GasT*Gauge	2.579	7	(8) + 2(7) + 8(5)
6 Operator*Gauge	2.252	8	(8) + 6(6)
7 GasT*Operator*Gauge	-3.780	8	(8) + 2(7)
8 Error	21.403		(8)

* Synthesized Test.

Error Terms for Synthesized Tests

Source	Error DF	Error MS	Synthesis of Error MS
1 GasT	6.97	222.63	(4) + (5) - (7)

Table 12-16 Minitab Balanced ANOVA for Example 12-7, Unrestricted Model

Analysis of Variance (Balanced Designs)

Factor	Type	Levels	Values			
GasT	fixed	3	60	75	90	
Operator	random	4	1	2	3	4
Gauge	random	3	1	2	3	

Analysis of Variance for Drop

Source	DF	SS	MS	F	P	
GasT	2	1023.36	511.68	2.30	0.171	x
Operator	3	423.82	141.27	0.63	0.616	x
Gauge	2	7.19	3.60	0.06	0.938	x
GasT*Operator	6	1211.97	202.00	14.59	0.000	
GasT*Gauge	4	137.89	34.47	2.49	0.099	
Operator*Gauge	6	209.47	34.91	2.52	0.081	
GasT*Operator*Gauge	12	166.11	13.84	0.65	0.788	
Error	36	770.50	21.40			
Total	71	3950.32				

x Not an exact F-test.

Source	Variance component	Error term	Expected Mean Square for Each Term (using unrestricted model)
1 GasT		*	(8) + 2(7) + 8(5) + 6(4) + Q[1]
2 Operator	-4.544	*	(8) + 2(7) + 6(6) + 6(4) + 18(2)
3 Gauge	-2.164	*	(8) + 2(7) + 6(6) + 8(5) + 24(3)
4 GasT*Operator	31.359	7	(8) + 2(7) + 6(4)
5 GasT*Gauge	2.579	7	(8) + 2(7) + 8(5)
6 Operator*Gauge	3.512	7	(8) + 2(7) + 6(6)
7 GasT*Operator*Gauge	-3.780	8	(8) + 2(7)
8 Error	21.403		(8)

* Synthesized Test.

Error Terms for Synthesized Tests

12-7 SOME ADDITIONAL TOPICS ON ESTIMATION OF VARIANCE COMPONENTS

As we have previously observed, estimating the variance components in a random or mixed model is frequently a subject of considerable importance to the experimenter. In this section, we present some further results and techniques useful in estimating variance components. We concentrate on procedures for finding confidence intervals on variance components, and we also illustrate how to find maximum likelihood estimates of variance components. The maximum likelihood method may be a useful alternative when the analysis of variance method produces negative estimates.

12-7.1 Approximate Confidence Intervals on Variance Components

When the random effects model was introduced in Section 12-1, we presented exact $100(1 - \alpha)$ percent confidence intervals for σ^2 and for other functions of the variance components in that simple experimental design. It is always possible to find an exact confidence interval on any function of the variance components that is the expected value of one of the mean squares in the analysis of variance. For example, consider the error mean square. Because $E(MS_E) = \sigma^2$, we can always find an exact confidence interval on σ^2 because the quantity

$$f_E MS_E/\sigma^2 = f_E\hat{\sigma}^2/\sigma^2$$

has a chi-square distribution with f_E degrees of freedom. The exact $100(1 - \alpha)$ percent confidence interval is

$$\frac{f_E MS_E}{\chi^2_{\alpha/2,f_E}} \leqslant \sigma^2 \leqslant \frac{f_E MS_E}{\chi^2_{1-\alpha/2,f_E}} \tag{12-36}$$

Unfortunately, in more complex experiments involving several design factors, it is generally not possible to find exact confidence intervals on the variance components of interest, because these variances are not the expected value of a single mean square from the analysis of variance. However, the concepts underlying Satterthwaite's approximate "pseudo" F tests, introduced in Section 12-6, can be employed to construct approximate confidence intervals on variance components for which no exact confidence interval is available.

Recall that Satterthwaite's method uses two linear combinations of mean squares

$$MS' = MS_r + \cdots + MS_s$$

and

$$MS'' = MS_u + \cdots + MS_v$$

with the test statistic

$$F = \frac{MS'}{MS''}$$

having an approximate F distribution. Using appropriate degrees of freedom for MS' and MS'', defined in Equations 12-34 and 12-35, this F statistic can be used in an approximate test of the significance of the parameter or variance component of interest.

For testing the significance of a variance component, say σ_0^2, the two linear combinations, MS' and MS'', are chosen such that the difference in their expected values is equal to a multiple of the component, say

$$E(MS') - E(MS'') = k\sigma_0^2$$

or

$$\sigma_0^2 = \frac{E(MS') - E(MS'')}{k}. \tag{12-37}$$

Equation 12-37 provides a basis for a point estimate of σ_0^2:

$$\begin{aligned}\hat{\sigma}_0^2 &= \frac{MS' - MS''}{k} \\ &= \frac{1}{k}MS_r + \cdots + \frac{1}{k}MS_s - \frac{1}{k}MS_u - \cdots - \frac{1}{k}MS_v\end{aligned} \tag{12-38}$$

The mean squares (MS_i) in Equation 12-38 are independent with $f_i MS_i/\sigma_i^2 = SS_i/\sigma_i^2$ having chi-square distributions with f_i degrees of freedom. The estimate of the variance component, $\hat{\sigma}_0^2$, is a linear combination of multiples of the mean squares, and $r\hat{\sigma}_0^2/\sigma_0^2$ has an approximate chi-square distribution with r degrees of freedom, where

$$\begin{aligned}r &= \frac{(\hat{\sigma}_0^2)^2}{\sum_{i=1}^{m}\frac{1}{k^2}\frac{MS_i^2}{f_i}} \\ &= \frac{(MS_r + \cdots + MS_s - MS_u - \cdots - MS_v)^2}{\frac{MS_r^2}{f_r} + \cdots + \frac{MS_s^2}{f_s} + \frac{MS_u^2}{f_u} + \cdots + \frac{MS_v^2}{f_v}}\end{aligned} \tag{12-39}$$

This result can only be used if $\hat{\sigma}_0^2 > 0$. As r will usually not be an integer, interpolation from the chi-square tables will generally be required. Graybill (1961) derives a general result for r.

Now because $r\hat{\sigma}_0^2/\sigma^2$ has an approximate chi-square distribution with r degrees of freedom,

$$P\left\{\chi_{1-\alpha/2,r}^2 \leq \frac{r\hat{\sigma}_0^2}{\sigma_0^2} \leq \chi_{\alpha/2,r}^2\right\} = 1 - \alpha$$

and

$$P\left\{\frac{r\hat{\sigma}_0^2}{\chi_{\alpha/2,r}^2} \leq \sigma_0^2 \leq \frac{r\hat{\sigma}_0^2}{\chi_{1-\alpha/2,r}^2}\right\} = 1 - \alpha$$

Therefore an approximate $100(1 - \alpha)$ percent confidence interval on σ_0^2 is

$$\frac{r\hat{\sigma}_0^2}{\chi_{\alpha/2,r}^2} \leq \sigma_0^2 \leq \frac{r\hat{\sigma}_0^2}{\chi_{1-\alpha/2,r}^2} \tag{12-40}$$

EXAMPLE 12-8

To illustrate this procedure, reconsider the experiment in Example 12-7, where a three-factor mixed model is used on a study of the pressure drop across an expansion valve of a turbine. The model is

$$y_{ijkl} = \mu + \tau_i + \beta_j + \gamma_k + (\tau\beta)_{ij} + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} + (\tau\beta\gamma)_{ijk} + \epsilon_{ijkl}$$

where τ_i is a fixed effect and all other effects are random. We will find an approximate confidence interval on $\sigma^2_{\tau\beta}$. Using the expected mean squares in Table 12-14, we note that the difference in the expected values of the mean squares for the two-way interaction effect AB and the three-way interaction effect ABC is a multiple of the variance component of interest, $\sigma^2_{\tau\beta}$:

$$\begin{aligned} E(MS_{AB}) - E(MS_{ABC}) &= \sigma^2 + n\sigma^2_{\tau\beta\gamma} + cn\sigma^2_{\tau\beta} - (\sigma^2 + n\sigma^2_{\tau\beta\gamma}) \\ &= cn\sigma^2_{\tau\beta} \end{aligned}$$

Therefore, the point estimate of $\sigma^2_{\tau\beta}$ is

$$\hat{\sigma}^2_{\tau\beta} = \frac{MS_{AB} - MS_{ABC}}{cn} = \frac{134.91 - 19.26}{(3)(2)} = 19.28$$

and

$$r = \frac{(MS_{AB} - MS_{ABC})^2}{\dfrac{MS^2_{AB}}{(a-1)(b-1)} + \dfrac{MS^2_{ABC}}{(a-1)(b-1)(c-1)}} = \frac{(134.91 - 19.26)^2}{\dfrac{(134.91)^2}{(2)(3)} + \dfrac{(19.26)^2}{(2)(3)(2)}} = 4.36$$

The approximate 95 percent confidence interval on $\sigma^2_{\tau\beta}$ is then found from Equation 12-40 as follows:

$$\frac{r\hat{\sigma}^2_{\tau\beta}}{\chi^2_{0.025,r}} \leq \sigma^2_{\tau\beta} \leq \frac{r\hat{\sigma}^2_{\tau\beta}}{\chi^2_{0.975,r}}$$

$$\frac{(4.36)(19.28)}{11.58} \leq \sigma^2_{\tau\beta} \leq \frac{(4.36)(19.28)}{0.61}$$

$$7.26 \leq \sigma^2_{\tau\beta} \leq 137.81$$

This result is consistent with the results of the exact F test on $\sigma^2_{\tau\beta}$, in that there is strong evidence that this variance component is not zero.

12-7.2 The Modified Large-Sample Method

The Satterthwaite method in the previous section is a relatively simple way to find an approximate confidence interval on a variance component that can be expressed as a linear combination of mean squares, say

$$\hat{\sigma}^2_0 = \sum_{i=1}^{Q} c_i MS_i \tag{12-41}$$

The Satterthwaite method works well when the degrees of freedom on each mean square MS_i are all relatively large, and when the constants c_i in Equation 12-41 are all positive. However, sometimes some of the c_i are negative. Graybill and Wang (1980) proposed a procedure called the **modified large-sample method**, which can be a very useful alternative to Satterthwaite's method. If all of the constants c_i in Equation 12-41 are positive, then the approximate $100(1 - \alpha)$ percent modified large-sample confidence interval on σ^2_0 is

$$\hat{\sigma}^2_0 - \sqrt{\sum_{i=1}^{Q} G_i^2 c_i^2 MS_i^2} \leq \sigma^2_0 \leq \hat{\sigma}^2_0 + \sqrt{\sum_{i=1}^{Q} H_i^2 c_i^2 MS_i^2} \tag{12-42}$$

where

$$G_i = 1 - \frac{1}{F_{\alpha,f_i,\infty}} \quad \text{and} \quad H_i = \frac{1}{F_{1-\alpha,f_i,\infty}} - 1$$

Note that an F random variable with an infinite number of denominator degrees of freedom is equivalent to a chi-square random variable divided by its degrees of freedom.

Now consider the more general case of Equation 12-41, where the constants c_i are unrestricted in sign. This may be written as

$$\hat{\sigma}_0^2 = \sum_{i=1}^{P} c_i MS_i - \sum_{j=P+1}^{Q} c_j MS_j, \qquad c_i, c_j \geqslant 0 \tag{12-43}$$

Ting et al. (1990) give an approximate $100(1 - \alpha)$ percent lower confidence limit on σ_0^2 as

$$L = \hat{\sigma}_0^2 - \sqrt{V_L} \tag{12-44}$$

where

$$V_L = \sum_{i=1}^{P} G_i^2 c_i^2 MS_i^2 + \sum_{j=P+1}^{Q} H_j^2 c_j^2 MS_j^2 + \sum_{i=1}^{P} \sum_{j=P+1}^{Q} G_{ij}^2 c_i c_j MS_i MS_j + \sum_{i=1}^{P-1} \sum_{t>i}^{P} G_{it}^* c_i c_t MS_i MS_t$$

$$G_i = 1 - \frac{1}{F_{\alpha,f_i,\infty}}$$

$$H_j = \frac{1}{F_{1-\alpha,f_i,\infty}} - 1$$

$$G_{ij} = \frac{(F_{\alpha,f_i,f_j} - 1)^2 - G_i^2 F_{\alpha,f_i,f_j}^2 - H_j^2}{F_{\alpha,f_i,f_j}}$$

$$G_{it}^* = \left[\left(1 - \frac{1}{F_{\alpha,f_i+f_t,\infty}} \right)^2 \frac{(f_i + f_t)^2}{f_i f_t} - \frac{G_i^2 f_i}{f_t} - \frac{G_t^2 f_t}{f_i} \right] (P - 1),$$

if $P > 1$ and $G_{it}^* = 0$ if $P = 1$

These results can also be extended to include approximate confidence intervals on ratios of variance components. For a complete account of these methods, refer to the excellent book by Burdick and Graybill (1992).

EXAMPLE 12-9

To illustrate the modified large-sample method, reconsider the three-factor mixed model in Example 12-7. We will find an approximate 95 percent lower confidence interval on $\sigma_{\tau\beta}^2$. Recall that the point estimate of $\sigma_{\tau\beta}^2$ is

$$\hat{\sigma}_{\tau\beta}^2 = \frac{MS_{AB} - MS_{ABC}}{cn} = \frac{134.91 - 19.26}{(3)(2)} = 19.28$$

Therefore, in the notation of Equation 12-43, $c_1 = c_2 = \frac{1}{6}$, and

$$G_1 = 1 - \frac{1}{F_{0.05,6,\infty}} = 1 - \frac{1}{2.1} = 0.524$$

$$H_2 = \frac{1}{F_{0.95,12,\infty}} - 1 = \frac{1}{0.435} - 1 = 1.30$$

$$G_{12} = \frac{(F_{0.05,6,12} - 1)^2 - (G_1)^2 F^2_{0.05,6,12} - (H_2)^2}{F_{0.05,6,12}}$$

$$= \frac{(3.00 - 1)^2 - (0.524)^2(3.00)^2 - (1.3)^2}{3.00} = -0.054$$

$$G^*_{1t} = 0$$

From Equation 12-44

$$V_L = G_1^2 c_1^2 MS_{AB}^2 + H_2^2 c_2^2 MS_{ABC}^2 + G_{12} c_1 c_2 MS_{AB} MS_{ABC}$$

$$= (0.524)^2(1/6)^2(134.91)^2 + (1.3)^2(1/6)^2(19.26)^2$$

$$+ (-0.054)(1/6)(1/6)(134.91)(19.26)$$

$$= 152.36$$

So an approximate 95 percent lower confidence limit on $\sigma^2_{\tau\beta}$ is

$$L = \hat{\sigma}^2_{\tau\beta} - \sqrt{V_L} = 19.28 - \sqrt{152.36} = 6.94$$

This result is consistent with the results of the exact F test for this effect.

12-7.3 Maximum Likelihood Estimation of Variance Components

This chapter has emphasized the analysis of variance method of variance component estimation because it is relatively straightforward and makes use of familiar quantities—the mean squares in the analysis of variance table. However, the method has some disadvantages, including an embarrassing tendency to produce negative estimates on occasion. Furthermore, the analysis of variance method is really a **method of moments estimator**, a technique that mathematical statisticians generally do not prefer to use for parameter estimation because it often results in parameter estimates that do not have good statistical properties. The preferred parameter estimation technique is called the **method of maximum likelihood**. The implementation of this method can be somewhat involved, particularly for an experimental design model, but in a sense, the method of maximum likelihood selects parameter estimates that, for a specified model and error distribution, maximize the probability of occurrence of the sample results. A very nice overview of the method of maximum likelihood applied to experimental design models is given by Milliken and Johnson (1984).

A complete presentation of the method of maximum likelihood is beyond the scope of this book, but the general idea can be illustrated very easily. Suppose that x is a random variable with probability distribution $f(x; \theta)$, where θ is an unknown parameter. Let x_1,

$x_2, \ldots, x_n$ be a random sample of n observations. Then the **likelihood function** of the sample is

$$L(\theta) = f(x_1;\ \theta) \cdot f(x_2;\ \theta) \cdot \cdots \cdot f(x_n;\ \theta)$$

Note that the likelihood function is now a function of only the unknown parameter θ. The maximum likelihood estimator of θ is the value of θ that maximizes the likelihood function $L(\theta)$.

To illustrate how this applies to an experimental design model with random effects, consider a two-factor model with $a = b = n = 2$. The model is

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \epsilon_{ijk}$$

with $i = 1, 2, j = 1, 2$, and $k = 1, 2$. The variance of any observation is

$$V(y_{ijk}) = \sigma_y^2 = \sigma_\tau^2 + \sigma_\beta^2 + \sigma_{\tau\beta}^2 + \sigma^2$$

and the covariances are

$$\begin{aligned} \text{Cov}(y_{ijk}, y_{i'j'k'}) &= \sigma_\tau^2 + \sigma_\beta^2 + \sigma_{\tau\beta}^2 && i = i', j = j', k \neq k' \\ &= \sigma_\tau^2 && i = i', j \neq j' \\ &= \sigma_\beta^2 && i \neq i', j = j' \\ &= 0 && i \neq i', j \neq j' \end{aligned} \tag{12-45}$$

It is convenient to think of the observations as an 8×1 vector, say

$$\mathbf{y} = \begin{bmatrix} y_{111} \\ y_{112} \\ y_{211} \\ y_{212} \\ y_{121} \\ y_{122} \\ y_{221} \\ y_{222} \end{bmatrix}$$

and the variances and covariances can be expressed as an 8×8 **covariance matrix**

$$\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix}$$

where $\boldsymbol{\Sigma}_{11}$, $\boldsymbol{\Sigma}_{22}$, $\boldsymbol{\Sigma}_{12}$ and $\boldsymbol{\Sigma}_{21} = \boldsymbol{\Sigma}_{12}'$ are 4×4 matrices defined as follows:

$$\boldsymbol{\Sigma}_{11} = \boldsymbol{\Sigma}_{22} = \begin{bmatrix} \sigma_y^2 & \sigma_\tau^2 + \sigma_\beta^2 + \sigma_{\tau\beta}^2 & \sigma_\tau^2 & \sigma_\tau^2 \\ \sigma_\tau^2 + \sigma_\beta^2 + \sigma_{\tau\beta}^2 & \sigma_y^2 & \sigma_\tau^2 & \sigma_\tau^2 \\ \sigma_\tau^2 & \sigma_\tau^2 & \sigma_y^2 & \sigma_\tau^2 + \sigma_\beta^2 + \sigma_{\tau\beta}^2 \\ \sigma_\tau^2 & \sigma_\tau^2 & \sigma_\tau^2 + \sigma_\beta^2 + \sigma_{\tau\beta}^2 & \sigma_y^2 \end{bmatrix}$$

$$\boldsymbol{\Sigma}_{12} = \begin{bmatrix} \sigma_\beta^2 & \sigma_\beta^2 & 0 & 0 \\ \sigma_\beta^2 & \sigma_\beta^2 & 0 & 0 \\ 0 & 0 & \sigma_\beta^2 & \sigma_\beta^2 \\ 0 & 0 & \sigma_\beta^2 & \sigma_\beta^2 \end{bmatrix}$$

and $\boldsymbol{\Sigma}_{21}$ is just the transpose of $\boldsymbol{\Sigma}_{12}$. Now each observation is normally distributed with variance σ_y^2, and if we assume that all $N = abn$ observations have a joint normal distribution, then the likelihood function for the random model becomes

$$L(\mu, \sigma_\tau^2, \sigma_\beta^2, \sigma_{\tau\beta}^2, \sigma^2) = \frac{1}{(2\pi)^{N/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{y} - \mathbf{j}_N\mu)'\boldsymbol{\Sigma}^{-1}(\mathbf{y} - \mathbf{j}_N\mu)\right]$$

where $\mathbf{j}_N$ is an $N \times 1$ vector of 1s. The maximum likelihood estimates of μ, σ_τ^2, σ_β^2, $\sigma_{\tau\beta}^2$, and σ^2 are those values of these parameters that maximize the likelihood function. It would also be desirable to restrict the variance component estimates to nonnegative values. So in practice, we would maximize the likelihood function subject to this constraint.

Estimating variance components by maximum likelihood requires specialized computer software. Some general statistical software packages have this capability. The SAS system computes maximum likelihood estimates of variance components in random or mixed models through SAS PROC MIXED. We will illustrate the use of PROC MIXED by applying it to the two-factor factorial model introduced in Examples 12-2 and 12-3.

First consider Example 12-2. The model is a two-factor factorial, random effects model. The analysis of variance method has produced a negative estimate of the interaction variance component. Negative estimates of variance components can be avoided in PROC MIXED by specifying that a **restricted** (or **residual**) **maximum likelihood** (**REML**) method be used. REML essentially constrains the variance component estimates to nonnegative values.

SAS PROC MIXED requires as input the covariance matrix of the model parameters. The structure for a random model where all the random variables are mutually independent is

$$\mathbf{G} = \begin{bmatrix} \sigma_\tau^2\mathbf{I} & 0 & 0 \\ 0 & \sigma_\beta^2\mathbf{I} & 0 \\ 0 & 0 & \sigma_{\tau\beta}^2\mathbf{I} \end{bmatrix} \tag{12-46}$$

where the $\mathbf{I}$'s are identity matrices. (The covariance structure of a model can be specified in PROC MIXED by the TYPE = *structure* option in the RANDOM statement. The covariance structure for the model in Example 12-2 is specified by TYPE = SIM (the default in PROC MIXED), which specifies the simple covariance structure for the model parameters given in Equation 12-46.

Table 12-17 (page 550) presents the output from SAS PROC MIXED for the experiment in Example 12-2. We specified the REML method of variance component estimation. The output has been annotated with numbers to facilitate the description shown below:

1. Variance component estimates and related output.
2. Covariance parameter. This identifies the model parameters: σ_τ^2, σ_β^2, $\sigma_{\tau\beta}^2$, and σ^2.
3. Ratio of estimated variance of effect to estimated residual error variance:

$$\hat{\sigma}_i^2/\hat{\sigma}^2$$

4. Parameter estimates. These are the REML estimates of the variance components $\hat{\sigma}_\tau^2$, $\hat{\sigma}_\beta^2$, $\hat{\sigma}_{\tau\beta}^2$, and $\hat{\sigma}^2$. Notice that the REML estimate of $\sigma_{\tau\beta}^2$ is zero.

Table 12-17 SAS PROC MIXED Output for Analysis of Gauge Repeatability and Reproducibility Study in Example 12-2 Using REML Estimation of Variance Components

The MIXED Procedure

Class Level Information

Class	Levels	Values
PART	20	1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
OPERATOR	3	1 2 3
REPLICAT	2	1 2

[1]

Covariance Parameter Estimates (REML)

[2] Cov Parm	[3] Ratio	[4] Estimate	[5] Std Errors	[6] Z	[7] Pr > |z|	[8] Alpha	[9] Lower	[9] Upper
OPERATOR	0.01203539	0.01062922	0.03286000	0.32	0.7463	0.05	-0.0538	0.0750
PART	11.60743820	10.25126446	3.37376878	3.04	0.0024	0.05	3.6388	16.8637
PART*OPERATOR	-0.00000000	-0.00000000	.	.	.	.	.	.
Residual	1.00000000	0.88316339	0.12616620	7.00	0.0000	0.05	0.6359	1.1304

[10]

Asymptotic Covariance Matrix of Estimates

Cov Parm	OPERATOR	PART	PART*OPERATOR	Residual
OPERATOR	0.00107978	0.00006632	0.00000000	-0.00039795
PART	0.00006632	11.38231579	0.00000000	-0.00265287
PART*OPERATOR	0.00000000	0.00000000	0.00000000	-0.00000000
Residual	-0.00039795	-0.00265287	-0.00000000	0.01591791

[11]

Model Fitting Information for VALUE

Description	Value
Observations	120.0000
Variance Estimate	0.8832
Standard Deviation Estimate	0.9398

Table 12-18 SAS PROC MIXED Output for Analysis of Gauge Repeatability and Reproducibility Study with the Operator as a Fixed Effect Using REML Estimation of Variance Components

The MIXED Procedure

Covariance Parameter Estimates (REML)

Cov Parm	Ratio	Estimate	Std Error	Z	Pr > |z|	Alpha	Lower	Upper
PART	11.60743876	10.25126472	3.37376895	3.04	0.0024	0.05	3.6388	16.8637
PART*OPERATOR	0.00000000	0.00000000	.	.	.	.	.	.
Residual	1.00000000	0.88316337	0.12616620	7.00	0.0000	0.05	0.6359	1.1304

Asymptotic Covariance Matrix of Estimates

Cov Parm	PART	PART*OPERATOR	Residual
PART	11.38231693	0.00000000	-0.00265287
PART*OPERATOR	0.00000000	0.00000000	-0.00000000
Residual	-0.00265287	0.00000000	-0.01591791

Model Fitting Information for VALUE

Description	Value
Observations	120.0000
Variance Estimate	0.8832
Standard Deviation Estimate	0.9398
REML Log Likelihood	-204.729
Akaike's Information Criterion	-207.729
Schwarz's Bayesian Criterion	-211.872
-2 REML Log Likelihood	409.4572

Tests of Fixed Effects

Source	NDF	DDF	Type III F	Pr > F
OPERATOR	2	38	1.48	0.2401

5. Standard error of estimate. This is the large-sample standard error of the parameter estimate; $se(\hat{\sigma}_i^2) = \sqrt{V(\hat{\sigma}_i^2)}$.
6. Z statistic associated with the estimated variance:

$$Z = \hat{\sigma}_i^2 / se(\hat{\sigma}_i^2).$$

7. P-value of the computed Z statistic.
8. Alpha level used to compute confidence interval.
9. Lower and upper bounds of a $100(1 - \alpha)$ percent large-sample normal theory confidence interval on the variance components:

$$L = \hat{\sigma}_i^2 - Z_{\alpha/2} se(\hat{\sigma}_i^2) \qquad U = \hat{\sigma}_i^2 + Z_{\alpha/2} se(\hat{\sigma}_i^2)$$

10. Asymptotic covariance matrix of estimates. This is the large-sample covariance matrix of the variance components estimates.
11. Model fitting measures for comparing the fit of alternative models.

Notice that the results from SAS PROC MIXED fairly closely match those reported in Example 12-2 when the reduced model (without the interaction term) was fit to the data.

In Example 12-3 we considered the same experiment but assumed that the operators were a fixed factor, leading to a mixed model. SAS PROC MIXED can be employed to estimate the variance components for this situation. The covariance structure for the observations, assuming that all random variables are mutually independent (that is, the unrestricted mixed model), is

$$\begin{aligned} \text{Cov}(y_{ijk}, y_{i'j'k'}) &= \sigma_\beta^2 + \sigma_{\tau\beta}^2 + \sigma^2 && i = i', j = j', k = k' \\ &= \sigma_\beta^2 + \sigma_{\tau\beta}^2 && i = i', j = j', k \neq k' \\ &= \sigma_\beta^2 && i \neq i', j = j' \\ &= 0 && j \neq j' \end{aligned} \tag{12-47}$$

The covariance matrix of the model parameters is

$$\mathbf{G} = \begin{bmatrix} \sigma_\beta^2 \mathbf{I} & 0 \\ 0 & \sigma_{\tau\beta}^2 \mathbf{I} \end{bmatrix} \tag{12-48}$$

(This is specified by the TYPE=SIM statement in the input to PROC MIXED.) The SAS PROC MIXED output for the unrestricted form of the mixed model of Example 12-3 is shown in Table 12-18 on the previous page. Once again, the REML method was selected. The estimate for the variance component for the factor "part" is very similar to the estimate obtained using the random model. The estimate for the residual error variance is also similar. In addition, the output includes an F test for the fixed effect.

12-8 PROBLEMS

12-1. A textile mill has a large number of looms. Each loom is supposed to provide the same output of cloth per minute. To investigate this assumption, five looms are chosen at random and their output is noted at different times. The following data are obtained:

Loom	Output (lb/min)				
1	14.0	14.1	14.2	14.0	14.1
2	13.9	13.8	13.9	14.0	14.0
3	14.1	14.2	14.1	14.0	13.9
4	13.6	13.8	14.0	13.9	13.7
5	13.8	13.6	13.9	13.8	14.0

(a) Explain why this is a random effects experiment. Are the looms equal in output? Use $\alpha = 0.05$.
(b) Estimate the variability between looms.
(c) Estimate the experimental error variance.
(d) Find a 95 percent confidence interval for $\sigma_\tau^2/(\sigma_\tau^2 + \sigma^2)$.
(e) Analyze the residuals from this experiment. Do you think that the analysis of variance assumptions are satisfied?

12-2. A manufacturer suspects that the batches of raw material furnished by his supplier differ significantly in calcium content. There are a large number of batches currently in the warehouse. Five of these are randomly selected for study. A chemist makes five determinations on each batch and obtains the following data:

Batch 1	Batch 2	Batch 3	Batch 4	Batch 5
23.46	23.59	23.51	23.28	23.29
23.48	23.46	23.64	23.40	23.46
23.56	23.42	23.46	23.37	23.37
23.39	23.49	23.52	23.46	23.32
23.40	23.50	23.49	23.39	23.38

(a) Is there significant variation in calcium content from batch to batch? Use $\alpha = 0.05$.
(b) Estimate the components of variance.
(c) Find a 95 percent confidence interval for $\sigma_\tau^2/(\sigma_\tau^2 + \sigma^2)$.
(d) Analyze the residuals from this experiment. Are the analysis of variance assumptions satisfied?

12-3. Several ovens in a metal working shop are used to heat metal specimens. All the ovens are supposed to operate at the same temperature, although it is suspected that this may not be true. Three ovens are selected at random and their temperatures on successive heats are noted. The data collected are as follows:

Oven	Temperature					
1	491.50	498.30	498.10	493.50	493.60	
2	488.50	484.65	479.90	477.35		
3	490.10	484.80	488.25	473.00	471.85	478.65

(a) Is there significant variation in temperature between ovens? Use $\alpha = 0.05$.
(b) Estimate the components of variance for this model.
(c) Analyze the residuals from this experiment and draw conclusions about model adequacy.

12-4. An article in the *Journal of the Electrochemical Society* (Vol. 139, No. 2, 1992, pp. 524–532) describes an experiment to investigate the low-pressure vapor deposition of polysilicon. The experiment was carried out in a large-capacity reactor at Sematech in Austin, Texas. The reactor has several wafer positions, and four of these positions are selected at random. The response variable is film thickness uniformity. Three replicates of the experiment were run, and the data are as follows:

Wafer Position	Uniformity		
1	2.76	5.67	4.49
2	1.43	1.70	2.19
3	2.34	1.97	1.47
4	0.94	1.36	1.65

(a) Is there a difference in the wafer positions? Use $\alpha = 0.05$.
(b) Estimate the variability due to wafer positions.
(c) Estimate the random error component.
(d) Analyze the residuals from this experiment and comment on model adequacy.

12-5. Consider the vapor-deposition experiment described in Problem 12-4.
(a) Estimate the total variability in the uniformity response.
(b) How much of the total variability in the uniformity response is due to the difference between positions in the reactor?
(c) To what level could the variability in the uniformity response be reduced if the position-to-position variability in the reactor could be eliminated? Do you believe this is a significant reduction?

12-6. An article in the *Journal of Quality Technology* (Vol. 13, No. 2, 1981, pp. 111–114) describes an experiment that investigates the effects of four bleaching chemicals on pulp brightness. These four chemicals were selected at random from a large population of potential bleaching agents. The data are as follows:

Chemical	Pulp Brightness				
1	77.199	74.466	92.746	76.208	82.876
2	80.522	79.306	81.914	80.346	73.385
3	79.417	78.017	91.596	80.802	80.626
4	78.001	78.358	77.544	77.364	77.386

(a) Is there a difference in the chemical types? Use $\alpha = 0.05$.
(b) Estimate the variability due to chemical types.
(c) Estimate the variability due to random error.
(d) Analyze the residuals from this experiment and comment on model adequacy.

12-7. Consider the one-way, balanced, random effects method. Develop a procedure for finding a $100(1 - \alpha)$ percent confidence interval for $\sigma^2/(\sigma_\tau^2 + \sigma^2)$.

12-8. Refer to Problem 12-1.
(a) What is the probability of accepting H_0 if σ_τ^2 is 4 times the error variance σ^2?
(b) If the difference between looms is large enough to increase the standard deviation of an observation by 20 percent, we wish to detect this with a probability of at least 0.80. What sample size should be used?

12-9. An experiment was performed to investigate the capability of a measurement system. Ten parts were randomly selected, and two randomly selected operators measured each part three times. The tests were made in random order, and the data below resulted.

Part Number	Operator 1 Measurements			Operator 2 Measurements		
	1	2	3	1	2	3
1	50	49	50	50	48	51
2	52	52	51	51	51	51
3	53	50	50	54	52	51
4	49	51	50	48	50	51
5	48	49	48	48	49	48
6	52	50	50	52	50	50
7	51	51	51	51	50	50
8	52	50	49	53	48	50
9	50	51	50	51	48	49
10	47	46	49	46	47	48

(a) Analyze the data from this experiment.
(b) Find point estimates of the variance components using the analysis of variance method.

12-10. Reconsider the data in Problem 5-6. Suppose that both factors, machines and operators, are chosen at random.
(a) Analyze the data from this experiment.
(b) Find point estimates of the variance components using the analysis of variance method.

12-11. Reconsider the data in Problem 5-13. Suppose that both factors are random.
(a) Analyze the data from this experiment.
(b) Estimate the variance components.

12-12. Suppose that in Problem 5-11 the furnace positions were randomly selected, resulting in a mixed model experiment. Reanalyze the data from this experiment under this new assumption. Estimate the appropriate model components.

12-13. Reanalyze the measurement systems experiment in Problem 12-9, assuming that operators are a fixed factor. Estimate the appropriate model components.

12-14. In Problem 5-6, suppose that there are only four machines of interest, but the operators were selected at random.
(a) What type of model is appropriate?
(b) Perform the analysis and estimate the model components.

12-15. By application of the expectation operator, develop the expected mean squares for the two-factor factorial, mixed model. Use the restricted model assumptions. Check your results with the expected mean squares given in Table 12-11 to see that they agree.

12-16. Consider the three-factor factorial design in Example 12-6. Propose appropriate test statistics for all main effects and interactions. Repeat for the case where A and B are fixed and C is random.

12-17. Consider the experiment in Example 12-7. Analyze the data for the case where A, B, and C are random.

12-18. Derive the expected mean squares shown in Table 12-14.

12-19. Consider a four-factor factorial experiment where factor A is at a levels, factor B is at b levels, factor C is at c levels, factor D is at d levels, and there are n replicates. Write down the sums of squares, the degrees of freedom, and the expected mean squares for the following cases. Assume the restricted model for all mixed models. You may use a computer package such as Minitab.
(a) A, B, C, and D are fixed factors.
(b) A, B, C, and D are random factors.
(c) A is fixed and B, C, and D are random.
(d) A and B are fixed and C and D are random.
(e) A, B, and C are fixed and D is random.
Do exact tests exist for all effects? If not, propose test statistics for those effects that cannot be directly tested.

12-20. Reconsider cases (c), (d), and (e) of Problem 12-19. Obtain the expected mean squares assuming the unrestricted model. You may use a computer package such as Minitab. Compare your results with those for the restricted model.

12-21. In Problem 5-17, assume that the three operators were selected at random. Analyze the data under these conditions and draw conclusions. Estimate the variance components.

12-22. Consider the three-factor factorial model

$$y_{ijk} = \mu + \tau_i + \beta_j + \gamma_k + (\tau\beta)_{ij} + (\beta\gamma)_{jk} + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, c \end{cases}$$

Assuming that all the factors are random, develop the analysis of variance table, including the expected mean squares. Propose appropriate test statistics for all effects.

12-23. The three-factor factorial model for a single replicate is

$$y_{ijk} = \mu + \tau_i + \beta_j + \gamma_k + (\tau\beta)_{ij} + (\beta\gamma)_{jk} + (\tau\gamma)_{ik} + (\tau\beta\gamma)_{ijk} + \epsilon_{ijk}$$

If all the factors are random, can any effects be tested? If the three-factor and $(\tau\beta)_{ij}$ interactions do not exist, can all the remaining effects be tested?

12-24. In Problem 5-6, assume that both machines and operators were chosen randomly. Determine the power of the test for detecting a machine effect such that $\sigma_\beta^2 = \sigma^2$, where σ_β^2 is the variance component for the machine factor. Are two replicates sufficient?

12-25. In the two-factor mixed model analysis of variance, show that $\text{Cov}[(\tau\beta)_{ij}, (\tau\beta)_{i'j}] = -(1/a)\sigma_{\tau\beta}^2$ for $i \neq i'$.

12-26. Show that the method of analysis of variance always produces unbiased point estimates of the variance components in any random or mixed model.

12-27. Invoking the usual normality assumptions, find an expression for the probability that a negative estimate of a variance component will be obtained by the analysis of variance method. Using this result, write a statement giving the probability that $\hat{\sigma}_\tau^2 < 0$ in a one-factor analysis of variance. Comment on the usefulness of this probability statement.

12-28. Analyze the data in Problem 12-9, assuming that operators are fixed, using both the unrestricted and the restricted forms of the mixed models. Compare the results obtained from the two models.

12-29. Consider the two-factor mixed model. Show that the standard error of the fixed factor mean (e.g., A) is $[MS_{AB}/bn]^{1/2}$.

12-30. Consider the variance components in the random model from Problem 12-9.
(a) Find an exact 95 percent confidence interval on σ^2.
(b) Find approximate 95 percent confidence intervals on the other variance components using the Satterthwaite method.

12-31. Use the experiment described in Problem 5-6 and assume that both factors are random. Find an exact 95 percent confidence interval on σ^2. Construct approximate 95 percent confidence intervals on the other variance components using the Satterthwaite method.

12-32. Consider the three-factor experiment in Problem 5-17 and assume that operators were selected at random. Find an approximate 95 percent confidence interval on the operator variance component.

12-33. Rework Problem 12-30 using the modified large-sample approach described in Section 12-7.2. Compare the two sets of confidence intervals obtained and discuss.

12-34. Rework Problem 12-32 using the modified large-sample method described in Section 12-7.2. Compare this confidence interval with the one obtained previously and discuss.

13 Nested and Split-Plot Designs

This chapter introduces two important types of experimental designs, the **nested design** and the **split-plot design**. Both of these designs find reasonably widespread application in the industrial use of designed experiments. They also frequently involve one or more **random factors**, and so some of the concepts introduced in Chapter 12 will find application here.

13-1 THE TWO-STAGE NESTED DESIGN

In certain multifactor experiments the levels of one factor (e.g., factor B) are similar but not identical for different levels of another factor (e.g., A). Such an arrangement is called a **nested**, or **hierarchical**, **design**, with the levels of factor B nested under the levels of factor A. For example, consider a company that purchases its raw material from three different suppliers. The company wishes to determine if the purity of the raw material is the same from each supplier. There are four batches of raw material available from each supplier, and three determinations of purity are to be taken from each batch. The situation is depicted in Figure 13-1 on the next page.

This is a **two-stage nested design**, with batches nested under suppliers. At first glance, you may ask why this is not a factorial experiment. If this were a factorial, then batch 1 would always refer to the same batch, batch 2 would always refer to the same batch, and so on. This is clearly not the case because the batches from each supplier are **unique** for that particular supplier. That is, batch 1 from supplier 1 has no connection with batch 1 from any other supplier, batch 2 from supplier 1 has no connection with batch 2 from any other supplier, and so forth. To emphasize the fact that the batches from each supplier are different batches, we may renumber the batches as 1, 2, 3, and 4 from supplier 1; 5, 6, 7, and 8 from supplier 2; and 9, 10, 11, and 12 from supplier 3, as shown in Figure 13-2 on the next page.

Sometimes we may not know whether a factor is crossed in a factorial arrangement or nested. If the levels of the factor can be renumbered arbitrarily as in Figure 13-2, then the factor is nested.

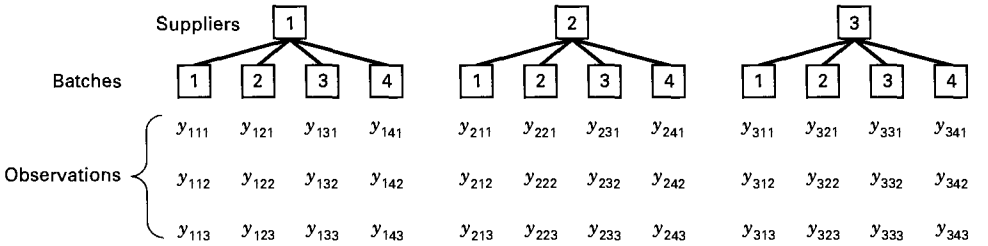


Figure 13-1 A two-stage nested design.

13-1.1 Statistical Analysis

The linear statistical model for the two-stage nested design is

$$y_{ijk} = \mu + \tau_i + \beta_{j(i)} + \epsilon_{(ij)k} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases} \tag{13-1}$$

That is, there are a levels of factor A, b levels of factor B nested under each level of A, and n replicates. The subscript $j(i)$ indicates that the jth level of factor B is nested under the ith level of factor A. It is convenient to think of the replicates as being nested within the combination of levels of A and B; thus, the subscript $(ij)k$ is used for the error term. This is a **balanced nested design** because there are an equal number of levels of B within each level of A and an equal number of replicates. Because every level of factor B does not appear with every level of factor A, there can be no interaction between A and B.

We may write the total corrected sum of squares as

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}(y_{ijk} - \bar{y}_{...})^2 = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}[(\bar{y}_{i..} - \bar{y}_{...}) + (\bar{y}_{ij.} - \bar{y}_{i..}) + (y_{ijk} - \bar{y}_{ij.})]^2 \tag{13-2}$$

Expanding the right-hand side of Equation 13-2 yields

$$\begin{aligned}\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}(y_{ijk} - \bar{y}_{...})^2 &= bn\sum_{i=1}^{a}(\bar{y}_{i..} - \bar{y}_{...})^2 + n\sum_{i=1}^{a}\sum_{j=1}^{b}(\bar{y}_{ij.} - \bar{y}_{i..})^2 \\ &\quad + \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n}(y_{ijk} - \bar{y}_{ij.})^2\end{aligned} \tag{13-3}$$

because the three cross-product terms are zero. Equation 13-3 indicates that the total sum of squares can be partitioned into a sum of squares due to factor A, a sum of squares due to factor B under the levels of A, and a sum of squares due to error. Symbolically, we may write Equation 13-3 as

$$SS_T = SS_A + SS_{B(A)} + SS_E \tag{13-4}$$

There are $abn - 1$ degrees of freedom for SS_T, $a - 1$ degrees of freedom for SS_A, $a(b - 1)$ degrees of freedom for $SS_{B(A)}$, and $ab(n - 1)$ degrees of freedom for error. Note that $abn - 1 = (a - 1) + a(b - 1) + ab(n - 1)$. If the errors are NID(0, σ^2), we may divide each sum of squares on the right of Equation 13-4 by its degrees of freedom

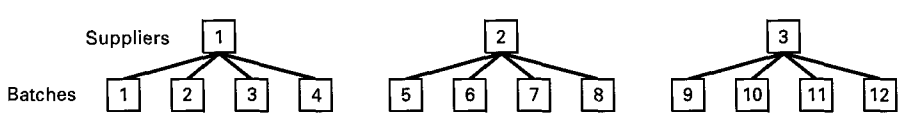


Figure 13-2 Alternate layout for the two-stage nested design.

Table 13-1 Expected Mean Squares in the Two-Stage Nested Design

$E(MS)$	A Fixed B Fixed	A Fixed B Random	A Random B Random
$E(MS_A)$	$\sigma^2 + \dfrac{bn\sum \tau_i^2}{a-1}$	$\sigma^2 + n\sigma_\beta^2 + \dfrac{bn\sum \tau_i^2}{a-1}$	$\sigma^2 + n\sigma_\beta^2 + bn\sigma_\tau^2$
$E(MS_{B(A)})$	$\sigma^2 + \dfrac{n\sum\sum \beta_{j(i)}^2}{a(b-1)}$	$\sigma^2 + n\sigma_\beta^2$	$\sigma^2 + n\sigma_\beta^2$
$E(MS_E)$	σ^2	σ^2	σ^2

to obtain independently distributed mean squares such that the ratio of any two mean squares is distributed as F.

The appropriate statistics for testing the effects of factors A and B depend on whether A and B are **fixed or random**. If factors A and B are fixed, we assume that $\sum_{i=1}^{a} \tau_i = 0$ and $\sum_{j=1}^{b} \beta_{j(i)} = 0$ $(i = 1, 2, \ldots, a)$. That is, the A treatment effects sum to zero, and the B treatment effects sum to zero within each level of A. Alternatively, if A and B are random, we assume that τ_i is NID$(0, \sigma_\tau^2)$ and $\beta_{j(i)}$ is NID$(0, \sigma_\beta^2)$. Mixed models with A fixed and B random are also widely encountered. The expected mean squares can be determined by a straightforward application of the rules in Chapter 12. For the mixed model, these expected mean squares assume the **restricted** form of the model in Chapter 12. Table 13-1 gives the expected mean squares for these situations.

Table 13-1 indicates that if the levels of A and B are fixed, $H_0: \tau_i = 0$ is tested by MS_A/MS_E and $H_0: \beta_{j(i)} = 0$ is tested by $MS_{B(A)}/MS_E$. If A is a fixed factor and B is random, then $H_0: \tau_i = 0$ is tested by $MS_A/MS_{B(A)}$ and $H_0: \sigma_\beta^2 = 0$ is tested by $MS_{B(A)}/MS_E$. Finally, if both A and B are random factors, we test $H_0: \sigma_\tau^2 = 0$ by $MS_A/MS_{B(A)}$ and $H_0: \sigma_\beta^2 = 0$ by $MS_{B(A)}/MS_E$. The test procedure is summarized in an analysis of variance table as shown in Table 13-2. Computing formulas for the sums of squares may be obtained by expanding the quantities in Equation 13-3 and simplifying. They are

$$SS_A = \frac{1}{bn}\sum_{i=1}^{a} y_{i..}^2 - \frac{y_{...}^2}{abn} \tag{13-5}$$

$$SS_{B(A)} = \frac{1}{n}\sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij.}^2 - \frac{1}{bn}\sum_{i=1}^{a} y_{i..}^2 \tag{13-6}$$

$$SS_E = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk}^2 - \frac{1}{n}\sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij.}^2 \tag{13-7}$$

$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk}^2 - \frac{y_{...}^2}{abn} \tag{13-8}$$

Table 13-2 Analysis of Variance Table for the Two-Stage Nested Design

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square
A	$bn\sum (\bar{y}_{i..} - \bar{y}_{...})^2$	$a - 1$	MS_A
B within A	$n\sum\sum (\bar{y}_{ij.} - \bar{y}_{i..})^2$	$a(b-1)$	$MS_{B(A)}$
Error	$\sum\sum\sum (y_{ijk} - \bar{y}_{ij.})^2$	$ab(n-1)$	MS_E
Total	$\sum\sum\sum (y_{ijk} - \bar{y}_{...})^2$	$abn - 1$	

We see that Equation 13-6 for $SS_{B(A)}$ can be written as

$$SS_{B(A)} = \sum_{i=1}^{a}\left[\frac{1}{n}\sum_{j=1}^{b} y_{ij.}^2 - \frac{y_{i..}^2}{bn}\right]$$

This expresses the idea that $SS_{B(A)}$ is the sum of squares between levels of B for each level of A, summed over all the levels of A.

EXAMPLE 13-1

Consider a company that buys raw material in batches from three different suppliers. The purity of this raw material varies considerably, which causes problems in manufacturing the finished product. We wish to determine if the variability in purity is attributable to differences between the suppliers. Four batches of raw material are selected at random from each supplier, and three determinations of purity are made on each batch. This is, of course, a two-stage nested design. The data, after coding by subtracting 93, are shown in Table 13-3. The sums of squares are computed as follows:

$$\begin{aligned}
SS_T &= \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk}^2 - \frac{y_{...}^2}{abn} \\
&= 153.00 - \frac{(13)^2}{36} = 148.31 \\
SS_A &= \frac{1}{bn}\sum_{i=1}^{a} y_{i..}^2 - \frac{y_{...}^2}{abn} \\
&= \frac{1}{(4)(3)}\left[(-5)^2 + (4)^2 + (14)^2\right] - \frac{(13)^2}{36} \\
&= 19.75 - 4.69 = 15.06 \\
SS_{B(A)} &= \frac{1}{n}\sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij.}^2 - \frac{1}{bn}\sum_{i=1}^{a} y_{i..}^2 \\
&= \frac{1}{3}\left[(0)^2 + (-9)^2 + (-1)^2 + \cdots + (2)^2 + (6)^2\right] - 19.75 \\
&= 89.67 - 19.75 = 69.92
\end{aligned}$$

and

$$\begin{aligned}
SS_E &= \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n} y_{ijk}^2 - \frac{1}{n}\sum_{i=1}^{a}\sum_{j=1}^{b} y_{ij.}^2 \\
&= 153.00 - 89.67 = 63.33
\end{aligned}$$

Table 13-3 Coded Purity Data for Example 13-1 (Code: y_{ijk} = purity − 93)

		Supplier 1				Supplier 2				Supplier 3			
	Batches	1	2	3	4	1	2	3	4	1	2	3	4
		1	−2	−2	1	1	0	−1	0	2	−2	1	3
		−1	−3	0	4	−2	4	0	3	4	0	−1	2
		0	−4	1	0	−3	2	−2	2	0	2	2	1
Batch totals	$y_{ij.}$	0	−9	−1	5	−4	6	−3	5	6	0	2	6
Supplier totals	$y_{i..}$		−5				4				14		

Table 13-4 Analysis of Variance for the Data in Example 13-1

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	Expected Mean Square	F_0	P-Value
Suppliers	15.06	2	7.53	$\sigma^2 + 3\sigma_\beta^2 + 6\sum \tau_i^2$	0.97	0.42
Batches (within suppliers)	69.92	9	7.77	$\sigma^2 + 3\sigma_\beta^2$	2.94	0.02
Error	63.33	24	2.64	σ^2		
Total	148.31	35				

The analysis of variance is summarized in Table 13-4. Suppliers are fixed and batches are random, so the expected mean squares are obtained from the middle column of Table 13-1. They are repeated for convenience in Table 13-4. From examining the P values, we would conclude that there is no significant effect on purity due to suppliers, but the purity of batches of raw material from the same supplier does differ significantly.

The practical implications of this experiment and the analysis are very important. The objective of the experimenter is to find the source of the variability in raw material purity. If it results from differences among suppliers, we may be able to solve the problem by selecting the "best" supplier. However, that solution is not applicable here because the major source of variability is the batch-to-batch purity variation *within* suppliers. Therefore, we must attack the problem by working with the suppliers to reduce their batch-to-batch variability. This may involve modifications to the suppliers' production processes or their internal quality assurance system.

Notice what would have happened if we had incorrectly analyzed this design as a two-factor factorial experiment. If batches are considered to be crossed with suppliers, we obtain batch totals of 2, −3, −2, and 16, with each batch × suppliers cell containing three replicates. Thus, a sum of squares due to batches and an interaction sum of squares can be computed. The complete factorial analysis of variance is shown in Table 13-5, assuming the mixed model.

This analysis indicates that batches differ significantly and that there is a significant interaction between batches and suppliers. However, it is difficult to give a practical interpretation of the batches × suppliers interaction. For example, does this significant interaction mean that the supplier effect is not constant from batch to batch? Furthermore, the significant interaction coupled with the nonsignificant supplier effect could lead the analyst to conclude that suppliers really differ but their effect is masked by the significant interaction.

Table 13-5 Incorrect Analysis of the Two-Stage Nested Design in Example 13-1 as a Factorial (Suppliers Fixed, Batches Random)

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Suppliers (S)	15.06	2	7.53	1.02	0.42
Batches (B)	25.64	3	8.55	3.24	0.04
$S \times B$ interaction	44.28	6	7.38	2.80	0.03
Error	63.33	24	2.64		
Total	148.31	35			

Computing

Some statistical software packages will perform the analysis for a nested design. Table 13-6 presents the output from the Balanced ANOVA procedure in Minitab (using the restricted model). The numerical results are in agreement with the manual calculations reported in Table 13-4. Minitab also reports the expected mean squares in the lower portion of Table 13-6. Remember that the symbol $Q[1]$ is a quadratic term that represents the fixed effect of suppliers, so in our notation,

$$Q[1] = \frac{\sum_{i=1}^{a} \tau_i^2}{a - 1}$$

Therefore, the fixed effect term in the Minitab expected mean square for suppliers $12Q[1] = 12\sum_{i=1}^{3} \tau_i^2/(3 - 1) = 6\sum_{i=1}^{3} \tau_i^2$, which matches the result given by the tabular algorithm in Table 13-4.

Sometimes a specialized computer program for analyzing nested designs is not available. However, notice from comparing Tables 13-4 and 13-5 that

$$SS_B + SS_{S\times B} = 25.64 + 44.28 = 69.92 \equiv SS_{B(S)}$$

That is, the sum of squares for batches within suppliers consist of the sum of squares of the batches plus the sum of squares for the batches × suppliers interaction. The degrees of freedom have a similar property; that is,

$$\frac{\text{Batches}}{3} + \frac{\text{Batches} \times \text{Suppliers}}{6} = \frac{\text{Batches within Suppliers}}{9}$$

Therefore, a computer program for analyzing factorial designs could also be used for the analysis of nested designs by pooling the "main effect" of the nested factor and interactions of that factor with the factor under which it is nested.

able 13-6 Minitab Output (Balanced ANOVA) for Example 13-1

nalysis of Variance (Balanced Designs)

```
actor              Type Levels Values
upplier           fixed      3      1      2      3
atch(Supplier) random       4      1      2      3      4

nalysis of Variance for Purity

ource              DF         SS         MS         F       P
upplier             2     15.056      7.528      0.97   0.416
atch(Supplier)      9     69.917      7.769      2.94   0.017
rror               24     63.333      2.639
otal               35    148.306

ource              Variance Error  Expected Mean Square for Each
                   component term  (using restricted model)
1 Supplier                    2    (3) + 3(2) + 12Q[1]
2 Batch(Supplier)     1.710   3    (3) + 3(2)
3 Error               2.639        (3)
```

13-1.2 Diagnostic Checking

The major tool used in diagnostic checking is **residual analysis**. For the two-stage nested design, the residuals are

$$e_{ijk} = y_{ijk} - \hat{y}_{ijk}$$

The fitted value is

$$\hat{y}_{ijk} = \hat{\mu} + \hat{\tau}_i + \hat{\beta}_{j(i)}$$

and if we make the usual restrictions on the model parameters ($\Sigma_i \hat{\tau}_i = 0$ and $\Sigma_j \hat{\beta}_{j(i)} = 0$, $i = 1, 2, \ldots, a$), then $\hat{\mu} = \bar{y}_{...}$, $\hat{\tau}_i = \bar{y}_{i..} - \bar{y}_{...}$, and $\hat{\beta}_{j(i)} = \bar{y}_{ij.} - \bar{y}_{i..}$. Consequently, the fitted value is

$$\begin{aligned}\hat{y}_{ijk} &= \bar{y}_{...} + (\bar{y}_{i..} - \bar{y}_{...}) + (\bar{y}_{ij.} - \bar{y}_{i..}) \\ &= \bar{y}_{ij.}\end{aligned}$$

Thus, the residuals from the two-stage nested design are

$$e_{ijk} = y_{ijk} - \bar{y}_{ij.} \tag{13-9}$$

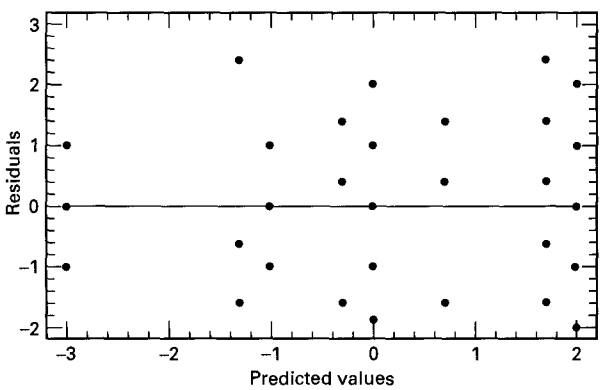
where $\bar{y}_{ij.}$ are the individual batch averages.

The observations, fitted values, and residuals for the purity data in Example 13-1 follow:

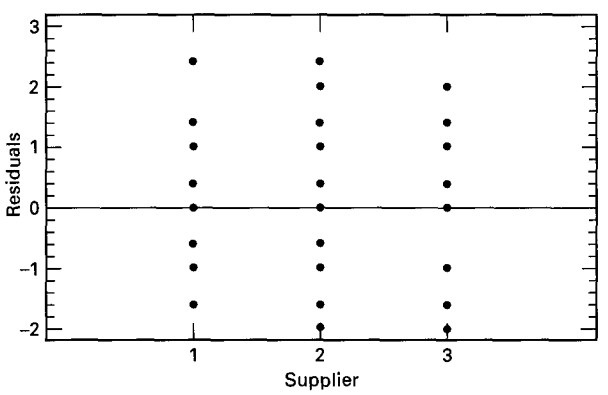
Observed Value y_{ijk}	Fitted Value $\hat{y}_{ijk} = \bar{y}_{ij.}$	$e_{ijk} = y_{ijk} - \bar{y}_{ij.}$
1	0.00	1.00
−1	0.00	−1.00
0	0.00	0.00
−2	−3.00	1.00
−3	−3.00	0.00
−4	−3.00	−1.00
−2	−0.33	−1.67
0	−0.33	0.33
1	−0.33	1.33
1	1.67	−0.67
4	1.67	2.33
0	1.67	−1.67
1	−1.33	2.33
−2	−1.33	−0.67
−3	−1.33	−1.67
0	2.00	−2.00
4	2.00	2.00
2	2.00	0.00
−1	−1.00	0.00
0	−1.00	1.00
−2	−1.00	−1.00
0	1.67	−1.67
3	1.67	1.33
2	1.67	0.33
2	2.00	0.00

Observed Value y_{ijk}	Fitted Value $\hat{y}_{ijk} = \bar{y}_{ij.}$	$e_{ijk} = y_{ijk} - \bar{y}_{ij.}$
4	2.00	2.00
0	2.00	−2.00
−2	0.00	−2.00
0	0.00	0.00
2	0.00	2.00
1	0.67	0.33
−1	0.67	−1.67
2	0.67	1.33
3	2.00	1.00
2	2.00	0.00
1	2.00	−1.00

The usual diagnostic checks—including normal probability plots, checking for outliers, and plotting the residuals versus fitted values—may now be performed. As an illustration, the residuals are plotted versus the fitted values and against the levels of the supplier factor in Figure 13-3.



(*a*) Plot of residuals versus the predicted values



(*b*) Plot of residuals versus supplier

Figure 13-3 Residual plots for Example 13-1.

In a problem situation such as that described in Example 13-1, the residual plots are particularly useful because of the additional diagnostic information they contain. For instance, the analysis of variance has indicated that the mean purity of all three suppliers does not differ but that there is statistically significant batch-to-batch variability (that is, $\sigma_\beta^2 > 0$). But is the variability within batches the same for all suppliers? In effect we have assumed this to be the case, and if it's not true we would certainly like to know it, because it has considerable practical impact on our interpretation of the results of the experiment. The plot of residuals versus suppliers in Figure 13-3*b* is a simple but effective way to check this assumption. Because the spread of the residuals is about the same for all three suppliers, we would conclude that the batch-to-batch variability in purity is about the same for all three suppliers.

13-1.3 Variance Components

For the random effects case, the analysis of variance method can be used to estimate the variance components σ^2,σ_β^2, and σ_τ^2. From the expected mean squares in the last column of Table 13-1, we obtain

$$\hat{\sigma}^2 = MS_E \tag{13-10}$$

$$\hat{\sigma}_\beta^2 = \frac{MS_{B(A)} - MS_E}{n} \tag{13-11}$$

and

$$\hat{\sigma}_\tau^2 = \frac{MS_A - MS_{B(A)}}{bn} \tag{13-12}$$

Many applications of nested designs involve a **mixed model**, with the main factor (A) fixed and the nested factor (B) random. This is the case for the problem described in Example 13-1; suppliers (factor A) are fixed, and batches of raw material (factor B) are random. The effects of the suppliers may be estimated by

$$\hat{\tau}_1 = \bar{y}_{1..} - \bar{y}_{...} = \frac{-5}{12} - \frac{13}{36} = \frac{-28}{36}$$

$$\hat{\tau}_2 = \bar{y}_{2..} - \bar{y}_{...} = \frac{4}{12} - \frac{13}{36} = \frac{-1}{36}$$

$$\hat{\tau}_3 = \bar{y}_{3..} - \bar{y}_{...} = \frac{14}{12} - \frac{13}{36} = \frac{29}{36}$$

To estimate the variance components σ^2 and σ_β^2, we eliminate the line in the analysis of variance table pertaining to suppliers and apply the analysis of variance estimation method to the next two lines. This yields

$$\hat{\sigma}^2 = MS_E = 2.64$$

and

$$\hat{\sigma}_\beta^2 = \frac{MS_{B(A)} - MS_E}{n} = \frac{7.77 - 2.64}{3} = 1.71$$

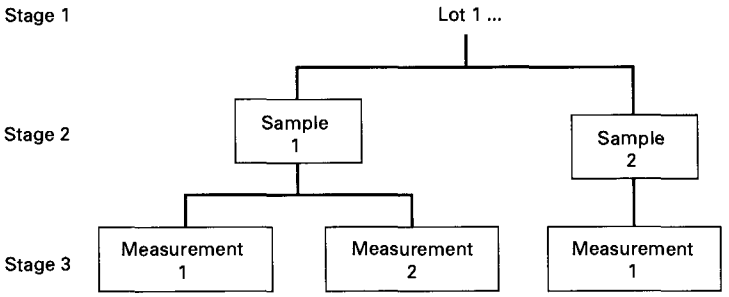


Figure 13-4 A three-stage staggered nested design.

These results are also shown in the lower portion of the Minitab output in Table 13-6. From the analysis in Example 13-1, we know that the τ_i do not differ significantly from zero, whereas the variance component σ_β^2 is greater than zero.

13-1.4 Staggered Nested Designs

A potential problem in the application of nested designs is that sometimes to get a reasonable number of degrees of freedom at the highest level, we can end up with many degrees of freedom (perhaps too many) at lower stages. To illustrate, suppose that we are investigating potential differences in chemical analysis among different lots of material. We plan to take five samples per lot, and each sample will be measured twice. If we want to estimate a variance component for lots, then 10 lots would not be an unreasonable choice. This results in 9 degrees of freedom for lots, 40 degrees of freedom for samples, and 50 degrees of freedom for measurements.

One way to avoid this is to use a particular type of unbalanced nested design called a **staggered nested design**. An example of a staggered nested design is shown in Figure 13-4. Notice that only two samples are taken from each lot; one of the samples is measured twice, whereas the other sample is measured once. If there are a lots, then there will be $a - 1$ degrees of freedom for lots (or, in general, the upper stage), and all lower stages will have exactly a degrees of freedom. For more information on the use and analysis of these designs, see Bainbridge (1965), Smith and Beverly (1981), Nelson (1983, 1995a, 1995b), and the supplemental text material for this chapter.

13-2 THE GENERAL m-STAGE NESTED DESIGN

The results of Section 13-1 can be easily extended to the case of m completely nested factors. Such a design would be called an ***m*-stage nested design**. As an example, suppose a foundry wishes to investigate the hardness of two different formulations of a metal alloy. Three heats of each alloy formulation are prepared, two ingots are selected at random from each heat for testing, and two hardness measurements are made on each ingot. The situation is illustrated in Figure 13-5 on the facing page.

In this experiment, heats are nested under the levels of the factor alloy formulation, and ingots are nested under the levels of the factor heats. Thus, this is a three-stage nested design with two replicates.

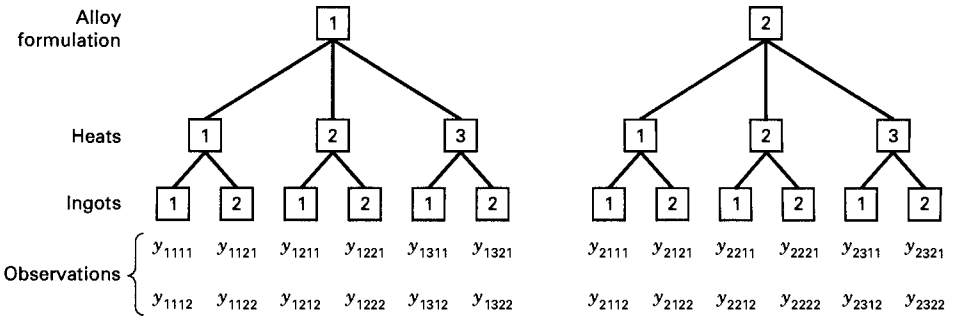


Figure 13-5 A three-stage nested design.

The **model** for the general three-stage nested design is

$$y_{ijkl} = \mu + \tau_i + \beta_{j(i)} + \gamma_{k(ij)} + \epsilon_{(ijk)l} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, c \\ l = 1, 2, \ldots, n \end{cases} \tag{13-13}$$

For our example, τ_i is the effect of the ith alloy formulation, $\beta_{j(i)}$ is the effect of the jth heat within the ith alloy, $\gamma_{k(ij)}$ is the effect of the kth ingot within the jth heat and ith

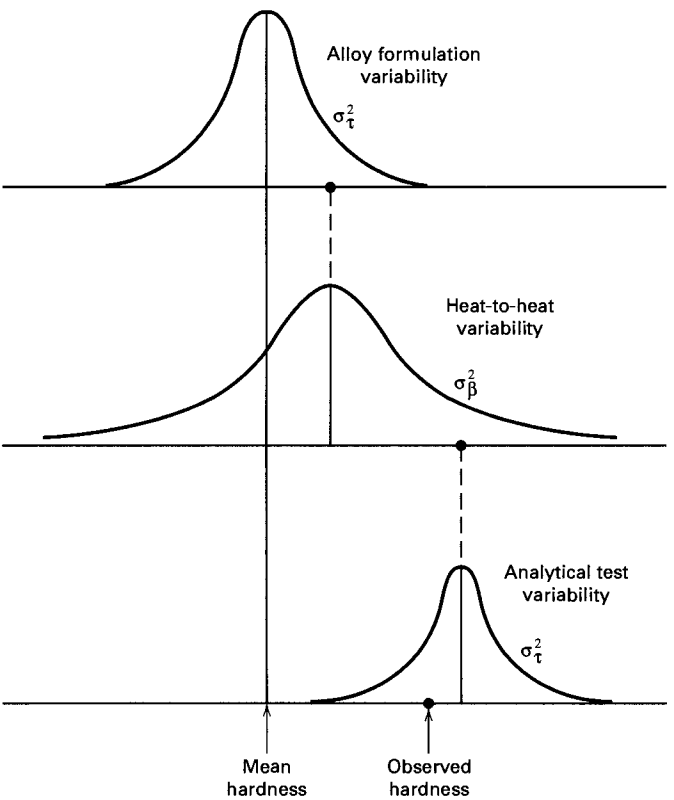


Figure 13-6 Sources of variation in the three-stage nested design example.

Table 13-7 Analysis of Variance for the Three-Stage Nested Design

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square
A	$bcn\sum_i(\bar{y}_{i...}-\bar{y}_{....})^2$	$a-1$	MS_A
B (within A)	$cn\sum_i\sum_j(\bar{y}_{ij..}-\bar{y}_{....})^2$	$a(b-1)$	$MS_{B(A)}$
C (within B)	$n\sum_i\sum_j\sum_k(\bar{y}_{ijk.}-\bar{y}_{....})^2$	$ab(c-1)$	$MS_{C(B)}$
Error	$\sum_i\sum_j\sum_k\sum_l(y_{ijkl}-\bar{y}_{ijk.})^2$	$abc(n-1)$	MS_E
Total	$\sum_i\sum_j\sum_k\sum_l(y_{ijkl}-\bar{y}_{....})^2$	$abcn-1$	

alloy, and $\epsilon_{(ijk)l}$ is the usual NID(0, σ^2) error term. Extension of this model to m factors is straightforward.

Notice that in the above example the overall variability in hardness consists of three components: one that results from alloy formulations, one that results from heats, and one that results from analytical test error. These components of the variability in overall hardness are illustrated in Figure 13-6 on the previous page.

This example demonstrates how the nested design is often used in analyzing processes to identify the major sources of variability in the output. For instance, if the alloy formulation variance component is large, then this implies that overall hardness variability could be reduced by using only one alloy formulation.

The calculation of the sums of squares and the analysis of variance for the m-stage nested design are similar to the analysis presented in Section 13-1. For example, the analysis of variance for the three-stage nested design is summarized in Table 13-7. Definitions of the sums of squares are also shown in this table. Notice that they are a simple extension of the formulas for the two-stage nested design. Many statistics software packages will perform the calculations.

To determine the proper test statistics we must find the expected mean squares using the methods of Chapter 12. For example, if factors A and B are fixed and factor C is random, then we may derive the expected mean squares as shown in Table 13-8. This table indicates the proper test statistics for this situation.

Table 13-8 Expected Mean Square Derivation for a Three-Stage Nested Design with A and B Fixed and C Random

	F	F	R	R	
	a	b	c	n	
Factor	i	j	k	l	Expected Mean Square
τ_i	0	b	c	n	$\sigma^2+n\sigma^2_\gamma+\dfrac{bcn\sum\tau_i^2}{a-1}$
$\beta_{j(i)}$	1	0	c	n	$\sigma^2+n\sigma^2_\gamma+\dfrac{cn\sum\sum\beta^2_{j(i)}}{a(b-1)}$
$\gamma_{k(ij)}$	1	1	1	n	$\sigma^2+n\sigma^2_\gamma$
$\epsilon_{l(ijk)}$	1	1	1	1	σ^2

13-3 DESIGNS WITH BOTH NESTED AND FACTORIAL FACTORS

Occasionally in a multifactor experiment, some factors are arranged in a factorial layout and other factors are nested. We sometimes call these designs **nested-factorial designs**. The statistical analysis of one such design with three factors is illustrated in the following example.

EXAMPLE 13-2

An industrial engineer is studying the hand insertion of electronic components on printed circuit boards to improve the speed of the assembly operation. He has designed three assembly fixtures and two workplace layouts that seem promising. Operators are required to perform the assembly, and it is decided to randomly select four operators for each fixture–layout combination. However, because the workplaces are in different locations within the plant, it is difficult to use the *same* four operators for each layout. Therefore, the four operators chosen for layout 1 are different individuals from the four operators chosen for layout 2. Because there are only three fixtures and two layouts, but the operators are chosen at random, this is a **mixed model**. The treatment combinations in this design are run in random order and two replicates are obtained. The assembly times are measured in seconds and are shown in Table 13-9.

In this experiment, operators are nested within the levels of layouts, whereas fixtures and layouts are arranged in a factorial. Thus, this design has both nested and factorial factors. The **linear model** for this design is

$$y_{ijkl} = \mu + \tau_i + \beta_j + \gamma_{k(j)} + (\tau\beta)_{ij} + (\tau\gamma)_{ik(j)} + \epsilon_{(ijk)l} \qquad \begin{cases} i = 1, 2, 3 \\ j = 1, 2 \\ k = 1, 2, 3, 4 \\ l = 1, 2 \end{cases} \tag{13-14}$$

where τ_i is the effect of the ith fixture, β_j is the effect of the jth layout, $\gamma_{k(j)}$ is the effect of the kth operator within the jth level of layout, $(\tau\beta)_{ij}$ is the fixture × layout interaction, $(\tau\gamma)_{ik(j)}$ is the fixture × operators within layout interaction, and $\epsilon_{(ijk)l}$ is the usual error term. Notice that no layout × operator interaction can exist because all the operators do not use all the layouts. Similarly, there can be no three-way fixture × layout × operator interaction. The expected mean squares are derived in Table 13-10 (page 570) using the tabular algorithm of Chapter 12. This produces a **restricted** mixed model analysis. The proper test statistic for any effect or interaction can be found from inspection of this table.

Table 13-9 Assembly Time Data for Example 13-2

	Layout 1				Layout 2				
Operator	1	2	3	4	1	2	3	4	$y_{i...}$
Fixture 1	22	23	28	25	26	27	28	24	404
	24	24	29	23	28	25	25	23	
Fixture 2	30	29	30	27	29	30	24	28	447
	27	28	32	25	28	27	23	30	
Fixture 3	25	24	27	26	27	26	24	28	401
	21	22	25	23	25	24	27	27	
Operator totals, $y_{.jk.}$	149	150	171	149	163	159	151	160	
Layout totals, $y_{.j..}$		619				633			$1252 = y_{....}$

Table 13-10 Expected Mean Square Derivation for Example 13-2

	F	F	R	R	
	3	2	4	2	
Factor	i	j	k	l	Expected Mean Square
τ_i	0	2	4	2	$\sigma^2 + 2\sigma^2_{\tau\gamma} + 8\sum \tau_i^2$
β_j	3	0	4	2	$\sigma^2 + 6\sigma^2_{\gamma} + 24\sum \beta_j^2$
$\gamma_{k(j)}$	3	1	1	2	$\sigma^2 + 6\sigma^2_{\gamma}$
$(\tau\beta)_{ij}$	0	0	4	2	$\sigma^2 + 2\sigma^2_{\tau\gamma} + 4\sum\sum (\tau\beta)^2_{ij}$
$(\tau\gamma)_{ik(j)}$	0	1	1	2	$\sigma^2 + 2\sigma^2_{\tau\gamma}$
$\epsilon_{(ijk)l}$	1	1	1	1	σ^2

The complete analysis of variance is shown in Table 13-11. We see that assembly fixtures are significant and that operators within layouts also differ significantly. There is also a significant interaction between fixtures and operators within layouts, indicating that the effects of the different fixtures are not the same for all operators. The workplace layouts seem to have little effect on the assembly time. Therefore, to minimize assembly time, we should concentrate on fixture types 1 and 3. (Note that the fixture totals in Table 13-9 are smaller for fixture types 1 and 3 than for type 2. This difference in fixture type means could be formally tested using multiple comparisons.) Furthermore, the interaction between operators and fixtures implies that some operators are more effective than others using the same fixtures. Perhaps these operator–fixture effects could be isolated and the less-effective operators' performance improved by retraining them.

Computing

There are a number of statistical software packages that can easily analyze nested-factorial designs, including both Minitab and SAS. Table 13-12 (page 571) presents the output from Minitab (Balanced ANOVA), assuming the restricted form of the mixed model, for Example 13-2. The expected mean squares in the bottom portion of Table 13-12 agree with those derived by the tabular method in Table 13-10. $Q[1]$, $Q[3]$, and $Q[4]$ are the fixed-factor effects for layouts, fixtures, and layouts × fixtures, respectively. The estimates of the variance components are:

Operator (layout): $\sigma^2_{\gamma} = 1.609$
Fixture × Operator (layout): $\sigma^2_{\tau\gamma} = 1.576$
Error: $\sigma^2 = 2.333$

Table 13-11 Analysis of Variance for Example 13-2

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Fixtures (F)	82.80	2	41.40	7.54	0.01
Layouts (L)	4.08	1	4.09	0.34	0.58
Operators (within layouts), $O(L)$	71.91	6	11.99	5.15	<0.01
FL	19.04	2	9.52	1.73	0.22
$FO(L)$	65.84	12	5.49	2.36	0.04
Error	56.00	24	2.33		
Total	299.67	47			

Table 13-12 Minitab Balanced ANOVA Analysis of Example 13-2 Using the Restricted Model

Analysis of Variance (Balanced Designs)

Factor	Type	Levels	Values			
Layout	fixed	2	1	2		
Operator(Layout)	random	4	1	2	3	4
Fixture	fixed	3	1	2	3	

Analysis of Variance for Time

Source	DF	SS	MS	F	P
Layout	1	4.083	4.083	0.34	0.581
Operator(Layout)	6	71.917	11.986	5.14	0.002
Fixture	2	82.792	41.396	7.55	0.008
Layout*Fixture	2	19.042	9.521	1.74	0.218
Fixture*Operator(Layout)	12	65.833	5.486	2.35	0.036
Error	24	56.000	2.333		
Total	47	299.667			

Source	Variance component	Error term	Expected Mean Square for Each Term (using restricted model)
1 Layout		2	(6) + 6(2) + 24Q[1]
2 Operator(Layout)	1.609	6	(6) + 6(2)
3 Fixture		5	(6) + 2(5) + 16Q[3]
4 Layout*Fixture		5	(6) + 2(5) + 8Q[4]
5 Fixture*Operator(Layout)	1.576	6	(6) + 2(5)
6 Error	2.333		(6)

Table 13-13 Minitab Balanced ANOVA Analysis of Example 13-2 Using the Unrestricted Model

Analysis of Variance (Balanced Designs)

Factor	Type	Levels	Values			
Layout	fixed	2	1	2		
Operator(Layout)	random	4	1	2	3	4
Fixture	fixed	3	1	2	3	

Analysis of Variance for Time

Source	DF	SS	MS	F	P
Layout	1	4.083	4.083	0.34	0.581
Operator(Layout)	6	71.917	11.986	2.18	0.117
Fixture	2	82.792	41.396	7.55	0.008
Layout*Fixture	2	19.042	9.521	1.74	0.218
Fixture*Operator(Layout)	12	65.833	5.486	2.35	0.036
Error	24	56.000	2.333		
Total	47	299.667			

Source	Variance component	Error term	Expected Mean Square for Each Term (using unrestricted model)
1 Layout		2	(6) + 2(5) + 6(2) + Q[1,4]
2 Operator(Layout)	1.083	5	(6) + 2(5) + 6(2)
3 Fixture		5	(6) + 2(5) + Q[3,4]
4 Layout*Fixture		5	(6) + 2(5) + Q[4]
5 Fixture*Operator(Layout)	1.576	6	(6) + 2(5)
6 Error	2.333		(6)

Table 13-13 (page 572) presents the Minitab analysis of Example 13-2 using the **unrestricted** form of the mixed model. The expected mean squares in the lower portion of this table are slightly different from those reported for the restricted model, and so the construction of the test statistic will be slightly different for the operators (layout) factor. Specifically, the F ratio denominator for operators (layout) is the fixtures $\times$ operators (layout) interaction in the restricted model (12 degrees of freedom for error), and it is the layout $\times$ fixtures interaction in the unrestricted model (2 degrees of freedom for error). Because $MS_{\text{layout}\times\text{fixture}} > MS_{\text{fixture}\times\text{operator(layout)}}$, and it has fewer degrees of freedom, we now find that the operator within layout effect is only significant at about the 12 percent level (the P value was 0.002 in the restricted model analysis). Furthermore, the variance component estimate $\hat{\sigma}^2_\gamma = 1.083$ is smaller. However, because there is a large fixture effect and a significant fixture $\times$ operator (layout) interaction, we would still suspect that there is an operator effect, and so the practical conclusions from this experiment are not greatly affected by choosing either the restricted or the unrestricted form of the mixed model. The quantities $Q[1, 4]$ and $Q[3, 4]$ are fixed-type quadratic terms containing the interaction effect of layouts $\times$ fixtures.

If there is no specialized software such as SAS or Minitab available, then a program for analyzing factorial experiments can be used to analyze experiments with nested and factorial factors. For instance, the experiment in Example 13-2 could be considered as a three-factor factorial, with fixtures (F), operators (O), and layouts (L) as the factors. Then certain sums of squares and degrees of freedom from the factorial analysis would be pooled to form the appropriate quantities required for the design with nested and factorial factors as follows:

Factorial Analysis		Nested-Factorial Analysis	
Sum of Squares	Degrees of Freedom	Sum of Squares	Degrees of Freedom
SS_F	2	SS_F	2
SS_L	1	SS_L	1
SS_{FL}	2	SS_{FL}	2
SS_O	3	$SS_{O(L)} = SS_O + SS_{LO}$	6
SS_{LO}	3		
SS_{FO}	6	$SS_{FO(L)} = SS_{FO} + SS_{FOL}$	12
SS_{FOL}	6		
SS_E	24	SS_E	24
SS_T	47	SS_T	47

13-4 THE SPLIT-PLOT DESIGN

In some multifactor factorial experiments we may be unable to completely randomize the order of the runs. This often results in a generalization of the factorial design called a **split-plot design**.

As an example, consider a paper manufacturer who is interested in three different pulp preparation methods and four different cooking temperatures for the pulp and who wishes to study the effect of these two factors on the tensile strength of the paper. Each replicate of a factorial experiment requires 12 observations, and the experimenter has

decided to run three replicates. However, the pilot plant is only capable of making 12 runs per day, so the experimenter decides to run one replicate on each of the three days and to consider the days or replicates as blocks. On any day, he conducts the experiment as follows. A batch of pulp is produced by one of the three methods under study. Then this batch is divided into four samples, and each sample is cooked at one of the four temperatures. Then a second batch of pulp is made up using another of the three methods. This second batch is also divided into four samples that are tested at the four temperatures. The process is then repeated, using a batch of pulp produced by the third method. The data are shown in Table 13-14.

Initially, we might consider this to be a factorial experiment with three levels of preparation method (factor A) and four levels of temperature (factor B) in a randomized block. If this is the case, then the order of experimentation within each replicate or block should be completely randomized. That is, within a block, we should randomly select a treatment combination (a preparation method and a temperature) and obtain an observation, then we should randomly select another treatment combination and obtain a second observation, and so on, until the 12 observations in the block have been taken. However, the experimenter did not collect the data this way. He made up a batch of pulp and obtained observations for all four temperatures from that batch. Because of the economics of preparing the batches and the size of the batches, this is the only feasible way to run this experiment. A completely randomized factorial experiment would require 36 batches of pulp, which is completely unrealistic. The split-plot design requires only three batches of pulp per block (replicate), in this case 9 batches total. Obviously, the split-plot design has resulted in considerable experimental efficiency.

The design used in our example is a split-plot design. Each replicate or block in the split-plot design is divided into three parts called **whole plots**, and the preparation methods are called the **whole plot** or **main treatments**. Each whole plot is divided into four parts called **subplots** (or **split-plots**), and one temperature is assigned to each. Temperature is called the **subplot treatment**. Note that if there are other uncontrolled or undesigned factors present, and if these uncontrolled factors vary as the pulp preparation methods are changed, then any effect of the undesigned factors on the response will be completely confounded with the effect of the pulp preparation methods. Because the whole plot treatments in a split-plot design are confounded with the whole plots and the subplot treatments are not confounded, it is best to assign the factor we are most interested in to the subplots, if possible.

This example is fairly typical of how the split-plot design is used in an industrial setting. Notice that the two factors were essentially "applied" at different times. Consequently, a split-plot design can be viewed as two experiments "combined" or super-

Table 13-14 The Experiment on the Tensile Strength of Paper

	Replicate (or Block) 1			Replicate (or Block) 2			Replicate (or Block) 3		
Pulp Preparation Method	1	2	3	1	2	3	1	2	3
Temperature (°F)									
200	30	34	29	28	31	31	31	35	32
225	35	41	26	32	36	30	37	40	34
250	37	38	33	40	42	32	41	39	39
275	36	42	36	41	40	40	40	44	45

imposed on each other. One "experiment" has the whole plot factor applied to the large experimental units (or it is a factor whose levels are hard to change) and the other "experiment" has the subplot factor applied to the smaller experimental units (or it is a factor whose levels are easy to change).

The **linear model** for the split-plot design is

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \gamma_k + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} + (\tau\beta\gamma)_{ijk} + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, r \\ j = 1, 2, \ldots, a \\ k = 1, 2, \ldots, b \end{cases} \tag{13-15}$$

where τ_i, β_j, and $(\tau\beta)_{ij}$ represent the whole plot and correspond respectively to blocks (or replicates), main treatments (factor A), and **whole plot error** (replicates (or blocks) $\times$ A); and γ_k, $(\tau\gamma)_{ik}$, $(\beta\gamma)_{jk}$, and $(\tau\beta\gamma)_{ijk}$ represent the subplot and correspond respectively to the subplot treatment (factor B), the replicates (or blocks) $\times$ B and AB interactions, and the **subplot error** (blocks $\times$ AB). Note that the whole plot error is the replicates (or blocks) $\times$ A interaction and the subplot error is the three-factor interaction blocks $\times$ AB. The sums of squares for these factors are computed as in the three-way analysis of variance without replication.

The expected mean squares for the split-plot design, with replicates or blocks random and main treatments and subplot treatments fixed, are derived in Table 13-15. Note that the main factor (A) in the whole plot is tested against the whole plot error, whereas the subtreatment (B) is tested against the replicates (or blocks) $\times$ subtreatment interaction. The AB interaction is tested against the subplot error. Notice that there are no tests for the replicate (or block) effect (A) or the replicate (or block) $\times$ subtreatment (AC) interaction.

The analysis of variance for the tensile strength data in Table 13-14 is summarized in Table 13-16 on the next page. Because both preparation methods and temperatures are fixed and replicates are random, the expected mean squares in Table 13-15 apply. The mean square for preparation methods is compared to the whole plot error mean

Table 13-15 Expected Mean Square Derivation for Split-Plot Design

		r	a	b	1	
		R	F	F	R	
	Factor	i	j	k	h	Expected Mean Square
Whole plot	τ_i	1	a	b	1	$\sigma^2 + ab\sigma^2_\tau$
	β_j	r	0	b	1	$\sigma^2 + b\sigma^2_{\tau\beta} + \dfrac{rb\sum \beta_j^2}{a-1}$
	$(\tau\beta)_{ij}$	1	0	b	1	$\sigma^2 + b\sigma^2_{\tau\beta}$
Subplot	γ_k	r	a	0	1	$\sigma^2 + a\sigma^2_{\tau\gamma} + \dfrac{ra\sum \gamma_k^2}{(b-1)}$
	$(\tau\gamma)_{ik}$	1	a	0	1	$\sigma^2 + a\sigma^2_{\tau\gamma}$
	$(\beta\gamma)_{jk}$	r	0	0	1	$\sigma^2 + \sigma^2_{\tau\beta\gamma} + \dfrac{r\sum\sum (\beta\gamma)^2_{jk}}{(a-1)(b-1)}$
	$(\tau\beta\gamma)_{ijk}$	1	0	0	1	$\sigma^2 + \sigma^2_{\tau\beta\gamma}$
	$\epsilon_{(ijk)h}$	1	1	1	1	σ^2 (not estimable)

Table 13-16 Analysis of Variance for the Split-Plot Design Using Tensile Strength Data from Table 13-14

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value
Replicates (or Blocks)	77.55	2	38.78		
Preparation method (A)	128.39	2	64.20	7.08	0.05
Whole Plot Error (replicates (or Blocks) × A)	36.28	4	9.07		
Temperature (B)	434.08	3	144.69	41.94	<0.01
Replicates (or Blocks) × B	20.67	6	3.45		
AB	75.17	6	12.53	2.96	0.05
Subplot Error (replicates (or Blocks) × AB)	50.83	12	4.24		
Total	822.97	35			

square, and the mean square for temperatures is compared to the replicate (or block) × temperature (AC) mean square. Finally, the preparation method × temperature mean square is tested against the subplot error. Both preparation methods and temperature have a significant effect on strength.

Note from Table 13-16 that the subplot error (4.24) is less than the whole plot error (9.07). This is the usual case in split-plot designs because the subplots are generally more homogeneous than the whole plots. This results in *two different error structures* for the experiment. Because the subplot treatments are compared with greater precision, it is preferable to assign the treatment we are most interested in to the subplots, if possible.

Some authors propose a slightly different statistical model for the split-plot design, say

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \gamma_k + (\beta\gamma)_{jk} + \epsilon_{ijk} \begin{cases} i = 1, 2, \ldots, r \\ j = 1, 2, \ldots, a \\ k = 1, 2, \ldots, b \end{cases} \quad (13\text{-}16)$$

In this model $(\tau\beta)_{ij}$ is still the whole plot error, but the blocks × B and blocks × AB interactions have essentially been pooled with ϵ_{ijk} to form the subplot error. If we denote the variance of the subplot error term ϵ_{ijk} by σ_ϵ^2 and make the same assumptions as for model (Equation 13-15), the expected mean squares become

Factor	$E(MS)$
τ_i (Replicates or Blocks)	$\sigma_\epsilon^2 + ab\sigma_\tau^2$
β_j (A)	$\sigma_\epsilon^2 + b\sigma_{\tau\beta}^2 + \dfrac{rb\sum \beta_j^2}{a-1}$
$(\tau\beta)_{ij}$	$\sigma_\epsilon^2 + b\sigma_{\tau\beta}^2$ (whole plot error)
γ_k (B)	$\sigma_\epsilon^2 + \dfrac{ra\sum \gamma_k^2}{ab-1}$
$(\beta\gamma)_{jk}$ (AB)	$\sigma_\epsilon^2 + \dfrac{r\sum\sum (\beta\gamma)_{jk}^2}{(a-1)(b-1)}$
ϵ_{ijk}	σ_ϵ^2 (subplot error)

Notice that now both the subplot treatment (B) and the AB interaction are tested against the subplot error mean square. If one is reasonably comfortable with the assumption that the replicates (or blocks) $\times$ B and replicates (or blocks) $\times$ AB interactions are negligible, then this alternative model is entirely satisfactory.

The split-plot design has an **agricultural heritage**, with the whole plots usually being large areas of land and the subplots being smaller areas of land within the large areas. For example, several varieties of a crop could be planted in different fields (whole plots), one variety to a field. Then each field could be divided into, say, four subplots, and each subplot could be treated with a different type of fertilizer. Here the crop varieties are the main treatments and the different fertilizers are the subtreatments.

Despite its agricultural basis, the split-plot design is useful in many scientific and industrial experiments. In these experimental settings, it is not unusual to find that some factors require large experimental units whereas other factors require small experimental units, such as in the tensile strength problem described above. Alternatively, we sometimes find that complete randomization is not feasible because it is more difficult to change the levels of some factors than others. The hard-to-vary factors form the whole plots whereas the easy-to-vary factors are run in the subplots.

In principle, we must carefully consider how the experiment must be conducted and incorporate all restrictions on randomization into the analysis. We illustrate this point using a modification of the eye focus time experiment in Chapter 6. Suppose there are only two factors, visual acuity (A) and illumination level (B). A factorial experiment with a levels of acuity, b levels of illumination, and n replicates would require that all abn observations be taken in random order. However, in the test apparatus, it is fairly difficult to adjust these two factors to different levels, so the experimenter decides to obtain the n replicates by adjusting the device to one of the a acuities and one of the b illumination levels and running all n observations at once. In the factorial design, the error actually represents the scatter or noise in the system plus the ability of the subject to reproduce the same focus time. The model for the factorial design could be written as

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \phi_{ijk} + \theta_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b \\ k = 1, 2, \ldots, n \end{cases} \tag{13-17}$$

where ϕ_{ijk} represents the scatter or noise in the system that results from "experimental error" (that is, our failure to duplicate exactly the same levels of acuity and illumination on different runs, variability in environmental conditions, and the like), and θ_{ijk} represents the "reproducibility error" of the subject. Usually, we combine these components into one overall error term, say $\epsilon_{ijk} = \phi_{ijk} + \theta_{ijk}$. Assume that $V(\epsilon_{ijk}) = \sigma^2 = \sigma_\phi^2 + \sigma_\theta^2$. Now, in the factorial design, the error mean square has expectation $\sigma^2 = \sigma_\phi^2 + \sigma_\theta^2$, with $ab(n - 1)$ degrees of freedom.

If we restrict the randomization as in the second design above, then the "error" mean square in the analysis of variance provides an estimate of the "reproducibility error" σ_θ^2 with $ab(n - 1)$ degrees of freedom, but it yields no information on the "experimental error" σ_ϕ^2. Thus, the mean square for error in this second design is too small; consequently, we will wrongly reject the null hypothesis very frequently. As pointed out by John (1971), this design is similar to a split-plot design with ab whole plots, each divided into n subplots, and no subtreatment. The situation is also similar to **subsam-**

pling, as described by Ostle (1963). Assuming that A and B are fixed, the expected mean squares in this case are

$$
\begin{aligned}
E(MS_A) &= \sigma_\theta^2 + n\sigma_\phi^2 + \frac{bn\sum \tau_i^2}{a-1} \\
E(MS_B) &= \sigma_\theta^2 + n\sigma_\phi^2 + \frac{an\sum \beta_j^2}{b-1} \\
E(MS_{AB}) &= \sigma_\theta^2 + n\sigma_\phi^2 + \frac{n\sum\sum (\tau\beta)_{ij}^2}{(a-1)(b-1)} \\
E(MS_E) &= \sigma_\theta^2
\end{aligned} \tag{13-18}
$$

Thus, there are no tests on the main effects unless interaction is negligible. The situation is exactly that of a two-way analysis of variance with one observation per cell. If both factors are random, then the main effects may be tested against the AB interaction. If only one factor is random, then the fixed factor can be tested against the AB interaction.

In general, if one analyzes a factorial design and all the main effects and interactions are significant, then one should examine carefully **how the experiment was actually conducted**. There may be randomization restrictions in the model not accounted for in the analysis, and consequently, the data should not be analyzed as a factorial.

13-5 OTHER VARIATIONS OF THE SPLIT-PLOT DESIGN

13-5.1 Split-Plot Designs with More Than Two Factors

Sometimes we find that either the whole plot or the subplot will contain two or more factors, arranged in a factorial structure. As an example, consider an experiment conducted on a furnace to grow an oxide on a silicon wafer. The response variables of interest are oxide layer thickness and layer uniformity. There are four design factors: temperature (A), gas flow (B), time (C), and wafer position in the furnace (D). The experimenter plans to run a 2^4 factorial design with two replicates (32 trials). Now factors A and B (temperature and gas flow) are difficult to change, whereas C and D (time and wafer position) are easy to change. This leads to the split-plot design shown in Figure 13-7 on the facing page. Notice that both replicates of the experiment are split into four whole plots, each containing one combination of the settings of temperature and gas flow. Once these levels are chosen, each whole plot is split into four subplots and a 2^2 factorial in the factors time and wafer position is conducted, where the treatment combinations in the subplot are tested in random order. Only four changes in temperature and gas flow are made in each replicate, whereas the levels of time and wafer position are completely randomized.

A model for this experiment, consistent with Equation 13-16, is

$$
\begin{aligned}
y_{ijklm} = {} & \mu + \tau_i + \beta_j + \gamma_k + (\beta\gamma)_{jk} + \theta_{ijk} + \delta_l + \lambda_m + (\delta\lambda)_{lm} \\
& + (\beta\delta)_{jl} + (\beta\lambda)_{jm} + (\gamma\delta)_{kl} + (\delta\lambda)_{lm} + (\beta\gamma\delta)_{jkl} + (\beta\gamma\lambda)_{jkm} \\
& + (\beta\delta\lambda)_{jlm} + (\gamma\delta\lambda)_{klm} + (\beta\gamma\delta\lambda)_{jklm} + \epsilon_{ijklm}
\end{aligned}
\qquad
\begin{cases} i = 1, 2 \\ j = 1, 2 \\ k = 1, 2 \\ l = 1, 2 \\ m = 1, 2 \end{cases} \tag{13-19}
$$

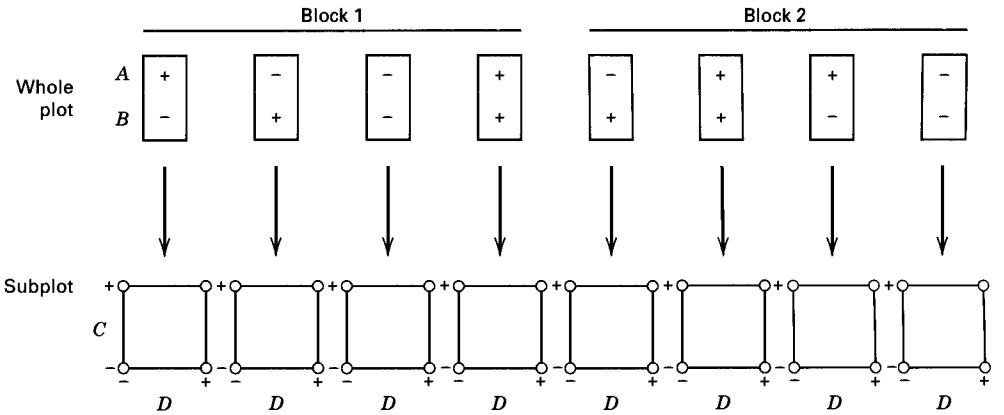


Figure 13-7 A split-plot design with four design factors, two in the whole plot and two in the subplot.

where τ_i represents the replicate effect, β_j and γ_k represent the whole plot main effects, θ_{ijk} is the whole plot error, δ_l and λ_m represent the subplot main effects, and ϵ_{ijklm} is the subplot error. We have included all interactions between the four design factors. Table 13-17 presents the analysis of variance for this design, assuming that replicates are random and all design factors are fixed effects. In this table σ_θ^2 and σ_ϵ^2 represent the variances of the whole plot and subplot errors, respectively, σ_τ^2 is the variance of the block

Table 13-17 An Abbreviated Analysis for a Split-Plot Design with Factors A and B in the Whole Plots and Factors C and D in the Subplots (Refer to Figure 13-7)

Source of Variation	Sum of Squares	Degrees of Freedom	Expected Mean Square
Replicates (τ_i)	$SS_{\text{Replicates}}$	1	$\sigma_\epsilon^2 + 16\sigma_\tau^2$
A (β_j)	SS_A	1	$\sigma_\epsilon^2 + 8\sigma_\theta^2 + A$
B (γ_k)	SS_B	1	$\sigma_\epsilon^2 + 8\sigma_\theta^2 + B$
AB	SS_{AB}	1	$\sigma_\epsilon^2 + 8\sigma_\theta^2 + AB$
Whole Plot Error (θ_{ijk})	SS_{WP}	3	$\sigma_\epsilon^2 + 8\sigma_\theta^2$
C (δ_l)	SS_C	1	$\sigma_\epsilon^2 + C$
D (λ_m)	SS_D	1	$\sigma_\epsilon^2 + D$
CD	SS_{CD}	1	$\sigma_\epsilon^2 + CD$
AC	SS_{AC}	1	$\sigma_\epsilon^2 + AC$
BC	SS_{BC}	1	$\sigma_\epsilon^2 + BC$
AD	SS_{AD}	1	$\sigma_\epsilon^2 + AD$
BD	SS_{BD}	1	$\sigma_\epsilon^2 + BD$
ABC	SS_{ABC}	1	$\sigma_\epsilon^2 + ABC$
ABD	SS_{ABD}	1	$\sigma_\epsilon^2 + ABD$
ACD	SS_{ACD}	1	$\sigma_\epsilon^2 + ACD$
BCD	SS_{BCD}	1	$\sigma_\epsilon^2 + BCD$
$ABCD$	SS_{ABCD}	1	$\sigma_\epsilon^2 + ABCD$
Subplot Error (ϵ_{ijklm})	SS_{SP}	12	σ_ϵ^2
Total	SS_T	31	

effects, and (for simplicity) we have used capital Latin letters to denote fixed-type effects. The whole plot main effects and interaction are tested against the whole plot error, whereas the subplot factors and all other interactions are tested against the subplot error. If some of the design factors are random, the test statistics will be different. In some cases there will be no exact F tests and Satterthwaite's procedure (described in Chapter 12) should be used.

Factorial experiments with three or more factors in a split-plot structure tend to be rather large experiments. On the other hand, the split-plot structure often makes it easier to conduct a larger experiment. For instance, in the oxide furnace example, the experimenters only have to change the hard-to-change factors (A and B) eight times, so perhaps a 32-run experiment is not too unreasonable. It is possible to reduce the number of runs by using a fractional factorial for the design factors of interest.

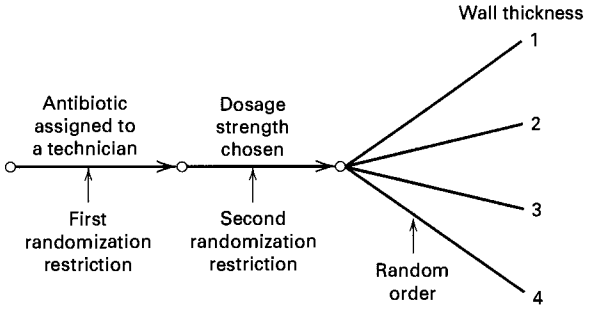
13-5.2 The Split-Split-Plot Design

The concept of split-plot designs can be extended to situations in which randomization restrictions may occur at any number of levels within the experiment. If there are two levels of randomization restrictions, the layout is called a **split-split-plot design**. The following example illustrates such a design.

EXAMPLE 13-3

A researcher is studying the absorption times of a particular type of antibiotic capsule. There are three technicians, three dosage strengths, and four capsule wall thicknesses of interest to the researcher. Each replicate of a factorial experiment would require 36 observations. The experimenter has decided on four replicates, and it is necessary to run each replicate on a different day. Note that the days can be considered as blocks. Within a replicate (or a block) (day), the experiment is performed by assigning a unit of antibiotic to a technician who conducts the experiment on the three dosage strengths and the four wall thicknesses. Once a particular dosage strength is formulated, all four wall thicknesses are tested at that strength. Then another dosage strength is selected and all four wall thicknesses are tested. Finally, the third dosage strength and the four wall thicknesses are tested. Meanwhile, two other laboratory technicians also follow this plan, each starting with a unit of antibiotic.

Note that there are *two* randomization restrictions within each replicate (or block): technician and dosage strength. The whole plots correspond to the technician. The order in which the technicians are assigned the units of antibiotic is randomly determined. The dosage strengths form three subplots. Dosage strength may be randomly assigned to a subplot. Finally, within a particular dosage strength, the four capsule wall thicknesses are tested in random order, forming four sub-subplots. The wall thicknesses are usually called sub-subtreatments. Because there are *two* randomization restrictions in the experiment (some authors say two "splits" in the design), the design is called a split-split-plot design. Figure 13-8 (page 581) illustrates the randomization restrictions and experimental layout in this design.



Blocks	Dosage strength	Technician 1			2			3		
		1	2	3	1	2	3	1	2	3
1	Wall thicknesses	1	1	1	1	1	1	1	1	1
		2	2	2	2	2	2	2	2	2
		3	3	3	3	3	3	3	3	3
		4	4	4	4	4	4	4	4	4
2	Wall thicknesses	1	1	1	1	1	1	1	1	1
		2	2	2	2	2	2	2	2	2
		3	3	3	3	3	3	3	3	3
		4	4	4	4	4	4	4	4	4
3	Wall thicknesses	1	1	1	1	1	1	1	1	1
		2	2	2	2	2	2	2	2	2
		3	3	3	3	3	3	3	3	3
		4	4	4	4	4	4	4	4	4
4	Wall thicknesses	1	1	1	1	1	1	1	1	1
		2	2	2	2	2	2	2	2	2
		3	3	3	3	3	3	3	3	3
		4	4	4	4	4	4	4	4	4

Figure 13-8 A split-split-plot design.

A linear statistical model for the split–split-plot design is

$$\begin{aligned} y_{ijkh} = {} & \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \gamma_k + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} + (\tau\beta\gamma)_{ijk} \\ & + \delta_h + (\tau\delta)_{ih} + (\beta\delta)_{jh} \\ & + (\tau\beta\delta)_{ijh} + (\gamma\delta)_{kh} + (\tau\gamma\delta)_{ikh} + (\beta\gamma\delta)_{jkh} \\ & + (\tau\beta\gamma\delta)_{ijkh} + \epsilon_{ijkh} \qquad \begin{cases} i = 1, 2, \ldots, r \\ j = 1, 2, \ldots, a \\ k = 1, 2, \ldots, b \\ h = 1, 2, \ldots, c \end{cases} \end{aligned} \tag{13-20}$$

where τ_i, β_j, and $(\tau\beta)_{ij}$ represent the whole plot and correspond to replicates or blocks, main treatments (factor A), and whole plot error (replicates (or blocks) $\times A$), respectively;

and γ_k, $(\tau\gamma)_{ik}$, $(\beta\gamma)_{jk}$ and $(\tau\beta\gamma)_{ijk}$ represent the subplot and correspond to the subplot treatment (factor B), the replicates (or blocks) $\times$ B and AB interactions, and the subplot error, respectively; and δ_h and the remaining parameters correspond to the sub-subplot and represent respectively the sub-subplot treatment (factor C) and the remaining interactions. The four-factor interaction $(\tau\beta\gamma\delta)_{ijkh}$ is called the sub-subplot error.

Assuming that the replicates (blocks) are random and that the other design factors are fixed, we may derive the expected mean squares as shown in Table 13-18. Tests on the main treatments, subtreatments, sub-subtreatments and their interactions are obvious from inspection of this table. Note that no tests on replicates or blocks or interactions involving replicates or blocks exist.

The statistical analysis of a split-split-plot design is like that of a single replicate of a four-factor factorial. The number of degrees of freedom for each test are determined in the usual manner. To illustrate, in Example 13-3, where we had four replicates, three technicians, three dosage strengths, and four wall thicknesses, we would have only $(r - 1)(a - 1) = (4 - 1)(3 - 1) = 6$ whole plot error degrees of freedom for testing technicians. This is a relatively small number of degrees of freedom, and the experimenter might consider using additional replicates to increase the precision of the test. If there are a replicates, we will have $2(r - 1)$ degrees of freedom for whole plot error. Thus,

Table 13-18 Expected Mean Square Derivation for the Split–Split-Plot Design

	Factor	r R i	a F j	b F k	c F h	1 R l	Expected Mean Square
Whole plot	τ_i	1	a	b	c	1	$\sigma^2 + abcd\sigma^2_\tau$
	β_j	r	0	b	c	1	$\sigma^2 + \sigma^2_{\tau\beta} + \dfrac{rbc\sum\beta_j^2}{(a-1)}$
	$(\tau\beta)_{ij}$	1	0	b	c	1	$\sigma^2 + bc\sigma^2_{\tau\beta}$
Subplot	γ_k	r	a	0	c	1	$\sigma^2 + ac\sigma^2_{\tau\gamma} + \dfrac{rac\sum\gamma_k^2}{(b-1)}$
	$(\tau\gamma)_{ik}$	1	a	0	c	1	$\sigma^2 + ac\sigma^2_{\tau\gamma}$
	$(\beta\gamma)_{jk}$	r	0	0	c	1	$\sigma^2 + c\sigma^2_{\tau\beta\gamma} + \dfrac{rc\sum\sum(\beta\gamma)^2_{jh}}{(a-1)(b-1)}$
	$\tau\beta\gamma)_{ijk}$	1	0	0	c	1	$\sigma^2 + c\sigma^2_{\tau\beta\gamma}$
Sub-subplot	δ_h	r	a	b	0	1	$\sigma^2 + ab\sigma^2_{\tau\delta} + \dfrac{rab\sum\delta_k^2}{(c-1)}$
	$(\tau\delta)_{ih}$	1	a	b	0	1	$\sigma^2 + ab\sigma^2_{\tau\delta}$
	$(\beta\delta)_{jh}$	r	0	b	0	1	$\sigma^2 + b\sigma^2_{\tau\beta\delta} + \dfrac{rb\sum\sum(\beta\delta)^2_{jh}}{(a-1)(c-1)}$
	$(\tau\beta\delta)_{ijh}$	1	0	b	0	1	$\sigma^2 + b\sigma^2_{\tau\beta\delta}$
	$(\gamma\delta)_{kh}$	r	a	0	0	1	$\sigma^2 + a\sigma^2_{\tau\gamma\delta} + \dfrac{ra\sum\sum(\gamma\delta)^2_{kh}}{(b-1)(c-1)}$
	$(\tau\gamma\delta)_{ikh}$	1	a	0	0	1	$\sigma^2 + a\sigma^2_{\tau\gamma\delta}$
	$(\beta\gamma\delta)_{jkh}$	r	0	0	0	1	$\sigma^2 + \sigma^2_{\tau\beta\gamma\delta} + \dfrac{r\sum\sum\sum(\beta\gamma\delta)^2_{ijk}}{(a-1)(b-1)(c-1)}$
	$(\tau\beta\gamma\delta)_{ijkh}$	1	0	0	0	1	$\sigma^2 + \sigma^2_{\tau\beta\gamma\delta}$
	$\epsilon_{l(ijkh)}$	1	1	1	1	1	σ^2 (not estimable)

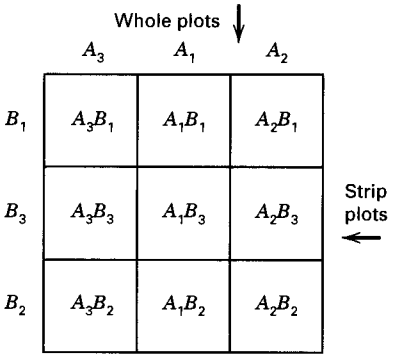


Figure 13-9 One replicate (block) of a strip-split-plot design.

five replicates yield $2(5 - 1) = 8$ error degrees of freedom, six replicates yield $2(6 - 1) = 10$ error degrees of freedom, seven replicates yield $2(7 - 1) = 12$ error degrees of freedom, and so on. Consequently, we would probably not want to run fewer than four replicates because this would yield only four error degrees of freedom. Each additional replicate allows us to gain two degrees of freedom for error. If we could afford to run five replicates, we could increase the precision of the test by one-third (from six to eight degrees of freedom). Also, in going from five to six replicates, there is an additional 25 percent gain in precision. If resources permit, the experimenter should run five or six replicates.

13-5.3 The Strip-Split-Plot Design

The strip-split-plot design has had extensive application in the agricultural sciences, but it finds occasional use in industrial experimentation. In the simplest case we have two factors A and B. Factor A is applied to whole plots just as in the standard split-plot design. Then factor B is applied to **strips** (which are really just another set of whole plots) that

Table 13-19 An Abbreviated Analysis of Variance for a Strip-Split-Plot Design

Source of Variation	Sum of Squares	Degrees of Freedom	Expected Mean Square
Replicates (or Blocks)	$SS_{\text{Replicates}}$	$r - 1$	$\sigma_\epsilon^2 + ab\sigma_\tau^2$
A	SS_A	$a - 1$	$\sigma_\epsilon^2 + b\sigma_{\tau\beta}^2 + \dfrac{rb\sum \beta_j^2}{a - 1}$
Whole Plot Error$_A$	SS_{WP_A}	$(r - 1)(a - 1)$	$\sigma_\epsilon^2 + b\sigma_{\tau\beta}^2$
B	SS_B	$b - 1$	$\sigma_\epsilon^2 + a\sigma_{\tau\gamma}^2 + \dfrac{ra\sum \gamma_k^2}{b - 1}$
Whole Plot Error$_B$	SS_{WP_B}	$(r - 1)(b - 1)$	$\sigma_\epsilon^2 + a\sigma_{\tau\gamma}^2$
AB	SS_{AB}	$(a - 1)(b - 1)$	$\sigma_\epsilon^2 + \dfrac{r\sum\sum (\tau\beta)_{jk}^2}{(a - 1)(b - 1)}$
Subplot Error	SS_{SP}	$(r - 1)(a - 1)(b - 1)$	σ_ϵ^2
Total	SS_T	$rab - 1$	

are orthogonal to the original whole plots used for factor A. Figure 13-9 (page 583) illustrates a situation in which both factors A and B have three levels. Note that the levels of factor A are confounded with the whole plots, and the levels of factor B are confounded with the strips (which can be thought of as a **second** set of whole plots).

A model for the strip-split plot design in Figure 13-9, assuming γ replicates, a levels of factor A, and b levels of factor B, is

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \gamma_k + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} + \epsilon_{ijk} \qquad \begin{cases} i = 1, 2, \ldots, r \\ j = 1, 2, \ldots, a \\ k = 1, 2, \ldots, b \end{cases}$$

where $(\tau\beta)_{ij}$ and $(\tau\gamma)_{ik}$ are whole plot errors for factors A and B, respectively, and ϵ_{ijk} is a "subplot" error, used to test the AB interaction. Table 13-19 (page 583) shows an abbreviated analysis of variance assuming A and B are fixed factors and replicates are random. The replicates are sometimes considered as blocks.

13-6 PROBLEMS

13-1. A rocket propellant manufacturer is studying the burning rate of propellant from three production processes. Four batches of propellant are randomly selected from the output of each process and three determinations of burning rate are made on each batch. The results follow. Analyze the data and draw conclusions.

	Process 1				Process 2				Process 3			
Batch	1	2	3	4	1	2	3	4	1	2	3	4
	25	19	15	15	19	23	18	35	14	35	38	25
	30	28	17	16	17	24	21	27	15	21	54	29
	26	20	14	13	14	21	17	25	20	24	50	33

13-2. The surface finish of metal parts made on four machines is being studied. An experiment is conducted in which each machine is run by three different operators and two specimens from each operator are collected and tested. Because of the location of the machines, different operators are used on each machine, and the operators are chosen at random. The data are shown in the following table. Analyze the data and draw conclusions.

	Machine 1			Machine 2			Machine 3			Machine 4		
Operator	1	2	3	1	2	3	1	2	3	1	2	3
	79	94	46	92	85	76	88	53	46	36	40	62
	62	74	57	99	79	68	75	56	57	53	56	47

13-3. A manufacturing engineer is studying the dimensional variability of a particular component that is produced on three machines. Each machine has two spindles, and four components are randomly selected from each spindle. The results follow. Analyze the data, assuming that machines and spindles are fixed factors.

	Machine 1		Machine 2		Machine 3	
Spindle	1	2	1	2	1	2
	12	8	14	12	14	16
	9	9	15	10	10	15
	11	10	13	11	12	15
	12	8	14	13	11	14

13-4. To simplify production scheduling, an industrial engineer is studying the possibility of assigning one time standard to a particular class of jobs, believing that differences between jobs are negligible. To see if this simplification is possible, six jobs are randomly selected. Each job is given to a different group of three operators. Each operator completes the job twice at different times during the week, and the following results are obtained. What are your conclusions about the use of a common time standard for all jobs in this class? What value would you use for the standard?

Job	Operator 1		Operator 2		Operator 3	
1	158.3	159.4	159.2	159.6	158.9	157.8
2	154.6	154.9	157.7	156.8	154.8	156.3
3	162.5	162.6	161.0	158.9	160.5	159.5
4	160.0	158.7	157.5	158.9	161.1	158.5
5	156.3	158.1	158.3	156.9	157.7	156.9
6	163.7	161.0	162.3	160.3	162.6	161.8

13-5. Consider the three-stage nested design shown in Figure 13-5 to investigate alloy hardness. Using the data that follow, analyze the design, assuming that alloy chemistry and heats are fixed factors and ingots are random. Use the restricted form of the mixed model.

	Alloy Chemistry											
Heats	1						2					
	1		2		3		1		2		3	
Ingots	1	2	1	2	1	2	1	2	1	2	1	2
	40	27	95	69	65	78	22	23	83	75	61	35
	63	30	67	47	54	45	10	39	62	64	77	42

13-6. Reanalyze the experiment in Problem 13-5 using the unrestricted form of the mixed model. Comment on any differences you observe between the restricted and the unrestricted model results. You may use a computer software package.

13-7. Derive the expected mean squares for a balanced three-stage nested design, assuming that A is fixed and that B and C are random. Obtain formulas for estimating the variance components. Assume the restricted form of the mixed model.

13-8. Repeat Problem 13-7 assuming the unrestricted form of the mixed model. You may use a computer software package to do this. Comment on any differences between the restricted and unrestricted model analysis and conclusions.

13-9. Derive the expected mean squares for a balanced three-stage nested design if all three factors are random. Obtain formulas for estimating the variance components.

13-10. Verify the expected mean squares given in Table 13-1.

13-11. ***Unbalanced nested designs.*** Consider an unbalanced two-stage nested design with b_j levels of B under the ith level of A and n_{ij} replicates in the ijth cell.

(a) Write down the least squares normal equations for this situation. Solve the normal equations.

(b) Construct the analysis of variance table for the unbalanced two-stage nested design.

(c) Analyze the following data, using the results in part (b):

Factor A	1		2		
Factor B	1	2	1	2	3
	6	−3	5	2	1
	4	1	7	4	0
	8		9	3	−3
			6		

13-12. ***Variance components in the unbalanced two-stage nested design.*** Consider the model

$$y_{ijk} = \mu + \tau_i + \beta_{j(i)} + \epsilon_{k(ij)} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, b_i \\ k = 1, 2, \ldots, n_{ij} \end{cases}$$

where A and B are random factors. Show that

$$\begin{aligned} E(MS_A) &= \sigma^2 + c_1\sigma_\beta^2 + c_2\sigma_\tau^2 \\ E(MS_{B(A)}) &= \sigma^2 + c_0\sigma_\beta^2 \\ E(MS_E) &= \sigma^2 \end{aligned}$$

where

$$c_0 = \frac{N - \sum_{i=1}^{a}\left(\sum_{j=1}^{b_i} n_{ij}^2/n_{i.}\right)}{b - a}$$

$$c_1 = \frac{\sum_{i=1}^{a}\left(\sum_{j=1}^{b_i} n_{ij}^2/n_{i.}\right) - \sum_{i=1}^{a}\sum_{j=1}^{b_i} n_{ij}^2/N}{a - 1}$$

$$c_2 = \frac{N - \dfrac{\sum_{i=1}^{a} n_{i.}^2}{N}}{a - 1}$$

13-13. A process engineer is testing the yield of a product manufactured on three machines. Each machine can be operated at two power settings. Furthermore, a machine has three stations on which the product is formed. An experiment is conducted in which each machine is tested at both power settings, and three observations on yield are taken from each station. The runs are made in random order, and the results follow. Analyze this experiment, assuming that all three factors are fixed.

	Machine 1			Machine 2			Machine 3		
Station	1	2	3	1	2	3	1	2	3
	34.1	33.7	36.2	31.1	33.1	32.8	32.9	33.8	33.6
Power setting 1	30.3	34.9	36.8	33.5	34.7	35.1	33.0	33.4	32.8
	31.6	35.0	37.1	34.0	33.9	34.3	33.1	32.8	31.7
	24.3	28.1	25.7	24.1	24.1	26.0	24.2	23.2	24.7
Power setting 2	26.3	29.3	26.1	25.0	25.1	27.1	26.1	27.4	22.0
	27.1	28.6	24.9	26.3	27.9	23.9	25.3	28.0	24.8

13-14. Suppose that in Problem 13-13 a large number of power settings could have been used and that the two selected for the experiment were chosen randomly. Obtain the expected mean squares for this situation assuming the restricted form of the mixed model and modify the previous analysis appropriately.

13-15. Reanalyze the experiment in Problem 13-14 assuming the unrestricted form of the mixed model. You may use a computer software package to do this. Comment on any differences between the restricted and unrestricted model analysis and conclusions.

13-16. A structural engineer is studying the strength of aluminum alloy purchased from three vendors. Each vendor submits the alloy in standard-sized bars of 1.0, 1.5, or 2.0 inches. The processing of different sizes of bar stock from a common ingot involves different forging techniques, and so this factor may be important. Furthermore, the bar stock is forged from ingots made in different heats. Each vendor submits two test specimens of each size bar stock from three heats. The resulting strength data follow. Analyze the data, assuming that vendors and bar size are fixed and heats are random. Use the restricted form of the mixed model.

	Vendor 1			Vendor 2			Vendor 3		
Heat	1	2	3	1	2	3	1	2	3
Bar size: 1 inch	1.230	1.346	1.235	1.301	1.346	1.315	1.247	1.275	1.324
	1.259	1.400	1.206	1.263	1.392	1.320	1.296	1.268	1.315
$1\frac{1}{2}$ inch	1.316	1.329	1.250	1.274	1.384	1.346	1.273	1.260	1.392
	1.300	1.362	1.239	1.268	1.375	1.357	1.264	1.265	1.364
2 inch	1.287	1.346	1.273	1.247	1.362	1.336	1.301	1.280	1.319
	1.292	1.382	1.215	1.215	1.328	1.342	1.262	1.271	1.323

13-17. Rework Problem 13-16 using the unrestricted form of the mixed model. You may use a computer software package to do this. Comment on any differences between the restricted and unrestricted model analysis and conclusions.

13-18. Suppose that in Problem 13-16 the bar stock may be purchased in many sizes and that the three sizes actually used in the experiment were selected randomly. Obtain the expected mean squares for this situation and modify the previous analysis appropriately. Use the restricted form of the mixed model.

13-19. Steel is normalized by heating above the critical temperature, soaking, and then air cooling. This process increases the strength of the steel, refines the grain, and homogenizes the structure. An experiment is performed to determine the effect of temperature and heat treatment time on the strength of normalized steel. Two temperatures and three

times are selected. The experiment is performed by heating the oven to a randomly selected temperature and inserting three specimens. After 10 minutes one specimen is removed, after 20 minutes the second is removed, and after 30 minutes the final specimen is removed. Then the temperature is changed to the other level and the process is repeated. Four shifts are required to collect the data, which are shown below. Analyze the data and draw conclusions, assuming both factors are fixed.

		Temperature, °F	
Shift	Time, minutes	1500	1600
	10	63	89
1	20	54	91
	30	61	62
	10	50	80
2	20	52	72
	30	59	69
	10	48	73
3	20	74	81
	30	71	69
	10	54	88
4	20	48	92
	30	59	64

13-20. An experiment is designed to study pigment dispersion in paint. Four different mixes of a particular pigment are studied. The procedure consists of preparing a particular mix and then applying that mix to a panel by three application methods (brushing, spraying, and rolling). The response measured is the percentage reflectance of pigment. Three days are required to run the experiment, and the data obtained follow. Analyze the data and draw conclusions, assuming that mixes and application methods are fixed.

	Application	Mix			
Day	Method	1	2	3	4
	1	64.5	66.3	74.1	66.5
1	2	68.3	69.5	73.8	70.0
	3	70.3	73.1	78.0	72.3
	1	65.2	65.0	73.8	64.8
2	2	69.2	70.3	74.5	68.3
	3	71.2	72.8	79.1	71.5
	1	66.2	66.5	72.3	67.7
3	2	69.0	69.0	75.4	68.6
	3	70.8	74.2	80.1	72.4

13-21. Repeat Problem 13-20, assuming that the mixes are random and the application methods are fixed.

13-22. Consider the split-split-plot design described in Example 13-3. Suppose that this experiment is conducted as described and that the data shown in the following table are obtained. Analyze the data and draw conclusions.

Replicates (or Blocks)	Dosage Strengths	Technician 1			2			3		
		1	2	3	1	2	3	1	2	3
	Wall Thickness									
	1	95	71	108	96	70	108	95	70	100
1	2	104	82	115	99	84	100	102	81	106
	3	101	85	117	95	83	105	105	84	113
	4	108	85	116	97	85	109	107	87	115
	1	95	78	110	100	72	104	92	69	101
2	2	106	84	109	101	79	102	100	76	104
	3	103	86	116	99	80	108	101	80	109
	4	109	84	110	112	86	109	108	86	113
	1	96	70	107	94	66	100	90	73	98
3	2	105	81	106	100	84	101	97	75	100
	3	106	88	112	104	87	109	100	82	104
	4	113	90	117	121	90	117	110	91	112
	1	90	68	109	98	68	106	98	72	101
4	2	100	84	112	102	81	103	102	78	105
	3	102	85	115	100	85	110	105	80	110
	4	114	88	118	118	85	116	110	95	120

13-23. Rework Problem 13-22, assuming that the technicians are chosen at random. Use the restricted form of the mixed model.

13-24. Suppose that in Problem 13-22 four technicians had been used. Assuming that all the factors are fixed, how many blocks should be run to obtain an adequate number of degrees of freedom on the test for differences among technicians?

13-25. Consider the experiment described in Example 13-3. Demonstrate how the order in which the treatment combinations are run would be determined if this experiment were run as (a) a split-split-plot, (b) a split-plot, (c) a factorial design in a randomized block, and (d) a completely randomized factorial design.

14 Other Design and Analysis Topics

The subject of statistically designed experiments is an extensive one. The previous chapters have provided an introductory presentation of many of the basic concepts and methods, yet in some cases, we have only been able to provide an overview. For example, there are book-length presentations of topics such as response surface methodology, mixture experiments, variance component estimation, and optimal design. In this chapter we provide an overview of several other topics that the experimenter may potentially find useful.

14-1 NONNORMAL RESPONSES AND TRANSFORMATIONS

14-1.1 Selecting a Transformation: The Box–Cox Method

In Section 3-4.3 we discussed the problem of nonconstant variance in the response variable y from a designed experiment and noted that this is a departure from the standard analysis of variance assumptions. This inequality of variance problem occurs relatively often in practice, often in conjunction with a nonnormal response variable. Examples would include a count of defects or particles, proportion data such as yield or fraction defective, or a response variable that follows some skewed distribution (one "tail" of the response distribution is longer than the other). We introduced **transformation of the response variable** as an appropriate method for stabilizing the variance of the response. Two methods for selecting the **form** of the transformation were discussed, an empirical graphical technique and essentially trial-and-error in which the experimenter simply tries one or more transformations, selecting the one that produces the most satisfactory or pleasing plot of residuals versus the fitted response.

Generally, transformations are used for three purposes; stabilizing response variance, making the distribution of the response variable closer to the normal distribution, and improving the fit of the model to the data. This last objective could include model simplification, say by eliminating interaction terms. Sometimes a transformation will

be reasonably effective in simultaneously accomplishing more than one of these objectives.

We have noted that the **power family** of transformations $y^* = y^\lambda$ is very useful, where λ is the parameter of the transformation to be determined (e.g., $\lambda = \frac{1}{2}$ means use the square root of the original response). Box and Cox (1964) have shown how the transformation parameter λ may be estimated simultaneously with the other model parameters (overall mean and treatment effects). The theory underlying their method uses the method of maximum likelihood. The actual computational procedure consists of performing, for various values of λ, a standard analysis of variance on

$$y^{(\lambda)} = \begin{cases} \dfrac{y^\lambda - 1}{\lambda \dot{y}^{\lambda-1}} & \lambda \neq 0 \\ \dot{y} \ln y & \lambda = 0 \end{cases} \tag{14-1}$$

where $\dot{y} = \ln^{-1}[(1/n) \Sigma \ln y]$ is the geometric mean of the observations. The maximum likelihood estimate of λ is the value for which the error sum of squares, say $SS_E(\lambda)$, is a minimum. This value of λ is usually found by plotting a graph of $SS_E(\lambda)$ versus λ and then reading the value of λ that minimizes $SS_E(\lambda)$ from the graph. Usually between 10 and 20 values of λ are sufficient for estimation of the optimum value. A second iteration using a finer mesh of values could be performed if a more accurate estimate of λ is necessary.

Notice that we *cannot* select the value of λ by *directly* comparing the error sums of squares from analyses of variance on y^λ because for each value of λ the error sum of squares is measured on a different scale. Furthermore, a problem arises in y when $\lambda = 0$; namely, as λ approaches zero, y^λ approaches unity.[5] That is, when $\lambda = 0$, all the response values are a constant. The component $(y^\lambda - 1)/\lambda$ of Equation 14-1 alleviates this problem because as λ tends to zero, $(y^\lambda - 1)/\lambda$ goes to a limit of $\ln y$. The divisor component $\dot{y}^{\lambda-1}$ in Equation 14-1 rescales the responses so that the error sums of squares are directly comparable.

In using the Box–Cox method, we recommend that the experimenter use simple choices for λ because the practical difference between $\lambda = 0.5$ and $\lambda = 0.58$ is likely to be small, but the square root transformation ($\lambda = 0.5$) is much easier to interpret. Obviously, values of λ close to unity would suggest that no transformation is necessary.

Once a value of λ is selected by the Box–Cox method, the experimenter can analyze the data using y^λ as the response, unless of course $\lambda = 0$, in which he can use $\ln y$. It is perfectly acceptable to use $y^{(\lambda)}$ as the actual response, although the model parameter estimates will have a scale difference and origin shift in comparison to the results obtained using y^λ (or $\ln y$).

An approximate $100(1 - \alpha)$ percent confidence interval for λ can be found by computing

$$SS^* = SS_E(\lambda)\left(1 + \frac{t^2_{\alpha/2,\nu}}{\nu}\right) \tag{14-2}$$

where ν is the number of degrees of freedom, and plotting a line parallel to the λ axis at height SS^* on the graph of $SS_E(\lambda)$ versus λ. Then by locating the points on the λ axis where SS^* cuts the curve $SS_E(\lambda)$, we can read confidence limits on λ directly from the graph. If this confidence interval includes the value $\lambda = 1$, this implies (as noted above) that the data do not support the need for transformation.

EXAMPLE 14-1

We will illustrate the Box–Cox procedure, using the peak discharge data originally presented in Example 3-5. Recall that this is a single-factor experiment (see Table 3-7 for the original data). Using Equation 14-1, we computed values of $SS_E(\lambda)$ for various values of λ:

λ	$SS_E(\lambda)$
−1.00	7922.11
−0.50	687.10
−0.25	232.52
0.00	91.96
0.25	46.99
0.50	35.42
0.75	40.61
1.00	62.08
1.25	109.82
1.50	208.12

A graph of values close to the minimum is shown in Figure 14-1 (on the facing page), from which it is seen that $\lambda \simeq 0.52$ gives a minimum value of approximately $SS_E(\lambda) = 35.00$. An approximate 95 percent confidence interval on λ is found by calculating the quantity SS^* from Equation 14-2 as follows:

$$SS^* = SS_E(\lambda)\left(1 + \frac{t^2_{0.025,20}}{20}\right)$$

$$= 35.00\left[1 + \frac{(2.086)^2}{20}\right]$$

$$= 42.61$$

By plotting SS^* on the graph in Figure 14-1 and by reading the points on the λ scale where this line intersects the curve, we obtain lower and upper confidence limits on λ of $\lambda^- = 0.27$ and $\lambda^+ = 0.77$. Because these confidence limits do not include the value 1, the use of a transformation is indicated, and the square root transformation ($\lambda = 0.50$) actually used is easily justified.

Some computer programs include the Box–Cox procedure for selecting a power family transformation. Figure 14-2 (on the facing page) presents the output from this procedure as implemented in Design-Expert for the peak discharge data. The results agree closely with the manual calculations summarized in Example 14-1. Notice that the vertical scale of the graph in Figure 14-2 is $\ln[SS_E(\lambda)]$.

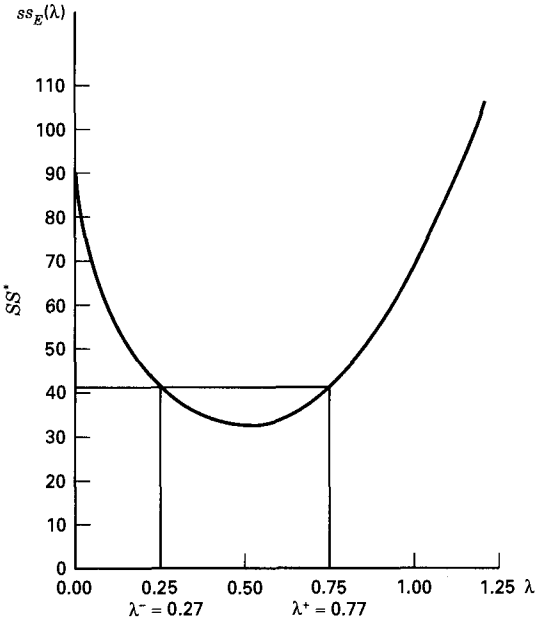


Figure 14-1 Plot of $SS_E(\lambda)$ versus λ for Example 14-1.

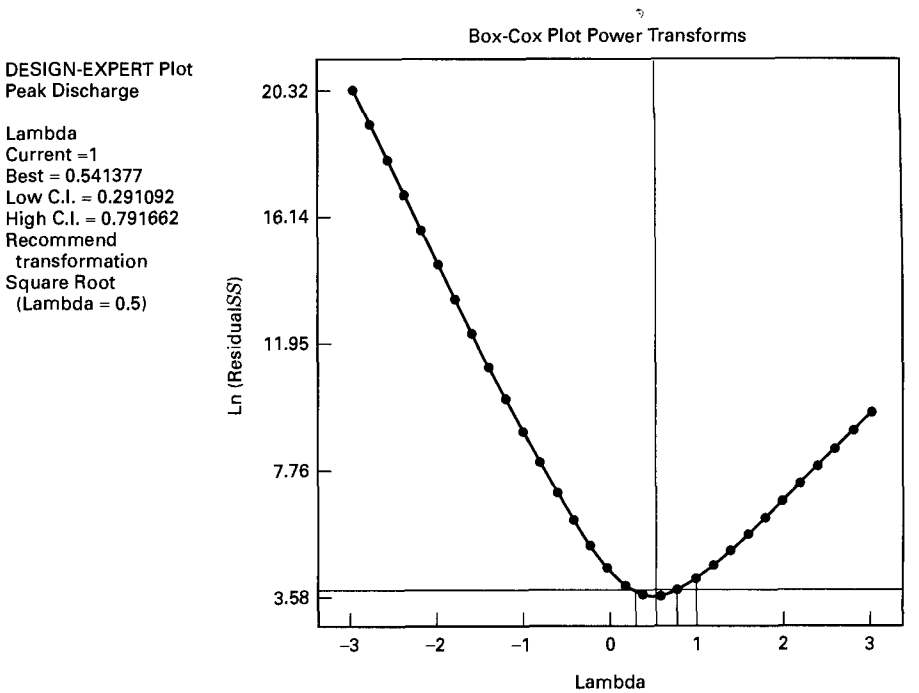


Figure 14-2 Output from Design-Expert for the Box–Cox procedure.

14-1.2 The Generalized Linear Model

Data transformations are often a very effective way to deal with the problem of nonnormal responses and the associated inequality of variance. As we have seen in the previous section, the Box–Cox method is an easy and effective way to select the form of the transformation. However, there can be problems associated with the use of a data transformation.

One problem is that the experimenter may be uncomfortable in working with the response in the transformed scale. That is, she is interested in the number of defects, not the *square root* of the number of defects, or in resistivity instead of the *logarithm* of resistivity. On the other hand, if a transformation is really successful and improves the analysis and the associated model for the response, experimenters will usually quickly adopt the new metric.

A more serious problem is that a transformation can result in a nonsensical value for the response variable over some portion of the design factor space that is of interest to the experimenter. For example, suppose that we have used the square root transformation in an experiment involving the number of defects observed on semiconductor wafers, and for some portion of the region of interest the predicted square root of the count of defects is negative. This is likely to occur for situations where the actual number of defects observed is small. Consequently, the model for the experiment has produced an obviously unreliable prediction in the very region where we would like this model to have good predictive performance.

Finally, as noted in Section 14-1.1, we often use transformations to stabilize variance, induce normality, and simplify the model. There is no assurance that a transformation will effectively accomplish all of these objectives simultaneously.

An alternative to the typical approach of data transformation followed by standard least squares analysis of the transformed response is to use the **generalized linear model**. This is an approach developed by Nelder and Wedderburn (1972) that essentially unifies linear and nonlinear models with both normal and nonnormal responses. McCullagh and Nelder (1989) give a comprehensive presentation of generalized linear models, and Myers and Montgomery (1997) provide a tutorial. More details are also given in the supplemental text material for this chapter. We will provide an overview of the concepts and illustrate them with two short examples.

A generalized linear model is basically a regression model (an experimental design model is also a regression model). Like all regression models, it is made up of a random component (what we have usually called the error term) and a function of the design factors (the x's) and some unknown parameters (the β's). In a standard normal-theory linear regression model we write

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \epsilon \tag{14-3}$$

where the error term ϵ is assumed to have a normal distribution with mean zero and constant variance, and the mean of the response variable y is

$$E(y) = \mu = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k = \mathbf{x}'\boldsymbol{\beta} \tag{14-4}$$

The portion $\mathbf{x}'\boldsymbol{\beta}$ of Equation (14-4) is called the **linear predictor**. The generalized linear model contains Equation (14-3) as a special case.

In a generalized linear model the response variable can have any distribution that is a member of the **exponential family**. This family includes the **normal**, **Poisson**, **bino-**

mial, **exponential**, and **gamma** distributions, so the exponential family is a very rich and flexible collection of distributions applicable to many experimental situations. Also, the relationship between the response mean μ and the linear predictor $\mathbf{x}'\boldsymbol{\beta}$ is determined by a **link function**.

$$g(\mu) = \mathbf{x}'\boldsymbol{\beta} \tag{14-5}$$

The regression model that represents the mean response is then given by

$$E(y) = \mu = g^{-1}(\mathbf{x}'\boldsymbol{\beta}) \tag{14-6}$$

For example, the link function leading to the ordinary linear regression model in Equation (14-3) is called the **identity link**, because $\mu = g^{-1}(\mathbf{x}'\boldsymbol{\beta}) = \mathbf{x}'\boldsymbol{\beta}$. As another example, the **log link**

$$\ln(\mu) = \mathbf{x}'\boldsymbol{\beta} \tag{14-7}$$

produces the model

$$\mu = e^{\mathbf{x}'\boldsymbol{\beta}} \tag{14-8}$$

The log link is often used with count data (Poisson response) and with continuous responses that have a distribution that has a long tail to the right (the exponential or gamma distribution). Another important link function used with binomial data is the **logit link**

$$\ln\left(\frac{\mu}{1-\mu}\right) = \mathbf{x}'\boldsymbol{\beta} \tag{14-9}$$

This choice of link function leads to the model

$$\mu = \frac{1}{1 + e^{\mathbf{x}'\boldsymbol{\beta}}} \tag{14-10}$$

There are many possible choices of link function, but it must always be monotonic and differentiable. Also note that in a generalized linear model, the variance of the response variable does not have to be a constant; it can be a function of the mean (and the predictor variables through the link function). For example, if the response is Poisson, the variance of the response is exactly equal to the mean.

To use a generalized linear model in practice, the experimenter must specify a response distribution and a link function. Then the model fitting or parameter estimation is done by the method of maximum likelihood, which for the exponential family turns out to be an iterative version of weighted least squares. For ordinary linear regression or experimental design models with a normal response variable, this reduces to standard least squares. Using an approach that is analogous to the analysis of variance for normal-theory data, we can perform inference and diagnostic checking for a generalized linear model. Refer to Myers and Montgomery (1997) for the details and examples. Two software packages that support the generalized linear model nicely are SAS (PROC GENMOD) and S-PLUS.

EXAMPLE 14-2

The Grill Defects Experiment

Problem 8-29 introduced an experiment to study the effects of nine factors on defects in sheet-molded grill opening panels. Bisgaard and Fuller (1994–1995) performed an interesting and useful analysis of this data to illustrate the value of data transformation in

Table 14-1 Least Squares and Generalized Linear Model Analysis for the Grill Opening Panels Experiment

	Using Least Squares Methods with Freeman and Tukey Modified Square Root Data Transformation				Generalized Linear Model (Poisson Response, Log Link)		Length of the 95% Confidence Interval	
	Transformed		Untransformed					
Observation	Predicted Value	95% Confidence Interval	Predicted Value	95% Confidence Interval	Predicted Value	95% Confidence Interval	Least Squares	GLM
1	5.50	(4.14, 6.85)	29.70	(16.65, 46.41)	51.26	(42.45, 61.90)	29.76	19.45
2	3.95	(2.60, 5.31)	15.12	(6.25, 27.65)	11.74	(8.14, 16.94)	21.39	8.80
3	1.52	(0.17, 2.88)	1.84	(1.69, 7.78)	1.12	(0.60, 2.08)	6.09	1.47
4	3.07	(1.71, 4.42)	8.91	(2.45, 19.04)	4.88	(2.87, 8.32)	16.59	5.45
5	1.52	(0.17, 2.88)	1.84	(1.69, 7.78)	1.12	(0.60, 2.08)	6.09	1.47
6	3.07	(1.71, 4.42)	8.91	(2.45, 19.04)	4.88	(2.87, 8.32)	16.59	5.45
7	5.50	(4.14, 6.85)	29.70	(16.65, 46.41)	51.26	(42.45, 61.90)	29.76	19.45
8	3.95	(2.60, 5.31)	15.12	(6.25, 27.65)	11.74	(8.14, 16.94)	21.39	8.80
9	1.08	(−0.28, 2.43)	0.71	(*, 5.41)	0.81	(0.42, 1.56)	*	1.13
10	−0.47	(−1.82, 0.89)	*	(*, 0.36)	0.19	(0.09, 0.38)	*	0.29
11	1.96	(0.61, 3.31)	3.36	(0.04, 10.49)	1.96	(1.16, 3.30)	10.45	2.14
12	3.50	(2.15, 4.86)	11.78	(4.13, 23.10)	8.54	(5.62, 12.98)	18.96	7.35
13	1.96	(0.61, 3.31)	3.36	(0.04, 10.49)	1.96	(1.16, 3.30)	10.45	2.14
14	3.50	(2.15, 4.86)	11.78	(4.13, 23.10)	8.54	(5.62, 12.98)	18.97	7.35
15	1.08	(−0.28, 2.43)	0.71	(*, 5.41)	0.81	(0.42, 1.56)	*	1.13
16	−0.47	(−1.82, 0.89)	*	(*, 0.36)	0.19	(0.09, 0.38)	*	0.29

a designed experiment. As we observed in Problem 8-29 part (f), they used a modification of the square root transformation that led to the model

$$\widehat{(\sqrt{y} + \sqrt{y+1})/2} = 2.513 - 0.996x_4 - 1.21x_6 - 0.772x_2x_7$$

where as usual, the x's represent the coded design factors. This transformation does an excellent job of stabilizing the variance of the number of defectives. The first two panels of Table 14-1 (page 596) present some information about this model. Under the "Transformed" heading, the first column contains the predicted response. Notice that there are two negative predicted values. The "untransformed" heading presents the untransformed predicted values, along with 95 percent confidence intervals on the mean response at each of the 16 design points. Because there were some negative predicted values, and negative lower confidence limits, we were unable to compute values for all of the entries in this panel of the table.

The response is essentially a square root of the count of defects. A negative predicted value is clearly illogical. Notice that this is occurring where the observed counts were small. If it is important to use the model to predict performance in this region, the model may be unreliable. This should *not* be taken as criticism of either the original experimenters or Bisgaard and Fuller's analysis. This was an extremely successful screening experiment that clearly defined the important processing variables. Prediction was not the original goal, nor was it the goal of the analysis done by Bisgaard and Fuller.

However, if obtaining a prediction model *had* been important, a generalized linear model would probably have been a good alternative to the transformation approach. Myers and Montgomery use a log link [Equation (14-7)] and Poisson response to fit exactly the same linear predictor given by Bisgaard and Fuller. This produces the model

$$\hat{y} = e^{(1.128 - 0.896x_4 - 1.176x_6 - 0.737x_2x_7)}$$

The third panel of Table 14-1 contains the predicted values from this model and the 95 percent confidence intervals on the mean response at each point in the design (obtained from SAS PROC GENMOD). There are no negative predicted values (assured by the choice of link function) and no negative lower confidence limits. The last panel of the table compares the lengths of the 95 percent confidence intervals for the untransformed response and the generalized linear model (GLM). Notice that the confidence intervals for the generalized linear model are uniformly *shorter* than their least squares counterparts. This is a strong indication that the generalized linear model approach has explained more variability and produced a superior model compared to the transformation approach.

EXAMPLE 14-3

The Worsted Yarn Experiment

Table 14-2 (page 598) presents a 3^3 factorial design conducted to investigate the performance of worsted yarn under cycles of repeated loading. The experiment is described thoroughly by Box and Draper (1987). The response is the number of cycles to failure. Reliability data such as this is typically nonnegative and continuous and often follows a distribution with a long right tail.

The data was initially analyzed using the standard (least squares) approach, and data transformation was necessary to stabilize the variance. The log of the cycles to failure

Table 14-2 The Worsted Yarn Experiment

Run	x_1	x_2	x_3	Cycles to Failure	Log Cycles to Failure
1	−1	−1	−1	674	2.83
2	−1	−1	0	370	2.57
3	−1	−1	1	292	2.47
4	−1	0	−1	338	2.53
5	−1	0	0	266	2.42
6	−1	0	1	210	2.32
7	−1	1	−1	170	2.23
8	−1	1	0	118	2.07
9	−1	1	1	90	1.95
10	0	−1	−1	1414	3.15
11	0	−1	0	1198	3.08
12	0	−1	1	634	2.8
13	0	0	−1	1022	3.01
14	0	0	0	620	2.79
15	0	0	1	438	2.64
16	0	1	−1	442	2.65
17	0	1	0	332	2.52
18	0	1	1	220	2.34
19	1	−1	−1	3636	3.56
20	1	−1	0	3184	3.5
21	1	−1	1	2000	3.3
22	1	0	−1	1568	3.19
23	1	0	0	1070	3.03
24	1	0	1	566	2.75
25	1	1	−1	1140	3.06
26	1	1	0	884	2.95
27	1	1	1	360	2.56

data is found to yield an adequate model in terms of overall model fit and satisfactory residual plots. The model is

$$\log \hat{y} = 2.751 + 0.3617x_1 - 0.2739x_2 - 0.1711x_3$$

or in terms of the original response, cycles to failure,

$$\hat{y} = 10^{2.751+0.3617x_1-0.2739x_2-0.1711x_3}.$$

This experiment was also analyzed using the generalized linear model, selecting the gamma response distribution and the log link. We used exactly the same model form found by least squares analysis of the log-transformed response. The model that resulted is

$$\hat{y} = e^{6.3489+0.8425x_1-0.6313x_2-0.3851x_3}.$$

Table 14-3 (on the facing page) presents the predicted values from the least squares model and the generalized linear model, along with 95 percent confidence intervals on the mean response at each of the 27 points in the design. A comparison of the lengths

Table 14-3 Least Squares and Generalized Linear Model Analysis for the Worsted Yarn Experiment

	Least Squares Methods with Log Data Transformation							
	Transformed		Untransformed		Generalized Linear Model		Length of the 95% Confidence Interval	
Obs.	Predicted Value	95% Confidence Interval	Predicted Value	95% Confidence Interval	Predicted Value	95% Confidence Interval	Least Squares	GLM
1	2.83	(2.76, 2.91)	682.50	(573.85, 811.52)	680.52	(583.83, 793.22)	237.67	209.39
2	2.66	(2.60, 2.73)	460.26	(397.01, 533.46)	463.00	(407.05, 526.64)	136.45	119.59
3	2.49	(2.42, 2.57)	310.38	(260.98, 369.06)	315.01	(271.49, 365.49)	108.09	94.00
4	2.56	(2.50, 2.62)	363.25	(313.33, 421.11)	361.96	(317.75, 412.33)	107.79	94.58
5	2.39	(2.34, 2.44)	244.96	(217.92, 275.30)	246.26	(222.55, 272.51)	57.37	49.96
6	2.22	(2.15, 2.28)	165.20	(142.50, 191.47)	167.55	(147.67, 190.10)	48.97	42.42
7	2.29	(2.21, 2.36)	193.33	(162.55, 229.93)	192.52	(165.69, 223.70)	67.38	58.01
8	2.12	(2.05, 2.18)	130.38	(112.46, 151.15)	130.98	(115.43, 148.64)	38.69	33.22
9	1.94	(1.87, 2.02)	87.92	(73.93, 104.54)	89.12	(76.87, 103.32)	30.62	26.45
10	3.20	(3.13, 3.26)	1569.28	(1353.94, 1819.28)	1580.00	(1390.00, 1797.00)	465.34	407.00
11	3.02	(2.97, 3.08)	1058.28	(941.67, 1189.60)	1075.00	(972.52, 1189.00)	247.92	216.48
12	2.85	(2.79, 2.92)	713.67	(615.60, 827.37)	731.50	(644.35, 830.44)	211.77	186.09
13	2.92	(2.87, 2.97)	835.41	(743.19, 938.86)	840.54	(759.65, 930.04)	195.67	170.39
14	2.75	(2.72, 2.78)	563.25	(523.24, 606.46)	571.87	(536.67, 609.38)	83.22	72.70
15	2.58	(2.53, 2.63)	379.84	(337.99, 426.97)	389.08	(351.64, 430.51)	88.99	78.87
16	2.65	(2.58, 2.71)	444.63	(383.53, 515.35)	447.07	(393.81, 507.54)	131.82	113.74
17	2.48	(2.43, 2.53)	299.85	(266.75, 336.98)	304.17	(275.13, 336.28)	70.23	61.15
18	2.31	(2.24, 2.37)	202.16	(174.42, 234.37)	206.95	(182.03, 235.27)	59.95	53.23
19	3.56	(3.48, 3.63)	3609.11	(3034.59, 4292.40)	3670.00	(3165.00, 4254.00)	1257.81	1089.00
20	3.39	(3.32, 3.45)	2433.88	(2099.42, 2821.63)	2497.00	(2200.00, 2833.00)	722.21	633.00
21	3.22	(3.14, 3.29)	1641.35	(1380.07, 1951.64)	1699.00	(1462.00, 1974.00)	571.57	512.00
22	3.28	(3.22, 3.35)	1920.88	(1656.91, 2226.90)	1952.00	(1720.00, 2215.00)	569.98	495.00
23	3.11	(3.06, 3.16)	1295.39	(1152.66, 1455.79)	1328.00	(1200.00, 1470.00)	303.14	270.00
24	2.94	(2.88, 3.01)	873.57	(753.53, 1012.74)	903.51	(793.15, 1029.00)	259.22	235.85
25	3.01	(2.93, 3.08)	1022.35	(859.81, 1215.91)	1038.00	(894.79, 1205.00)	356.10	310.21

of the confidence intervals reveals that the generalized linear model is likely to be a better predictor than the least squares model.

Generalized linear models have found extensive application in biomedical and pharmaceutical research and development. As more software packages incorporate this capability, it will find widespread application in the general industrial research and development environment.

14-2 UNBALANCED DATA IN A FACTORIAL DESIGN

The primary focus of this book has been the analysis of **balanced factorial designs**, that is, cases where there are an equal number of observations n in each cell. However, it is not unusual to encounter situations where the number of observations in the cells are unequal. These **unbalanced factorial designs** occur for various reasons. For example, the experimenter may have designed a balanced experiment initially, but because of unforeseen problems in running the experiment, resulting in the loss of some observations, he ends up with unbalanced data. On the other hand, some unbalanced experiments are deliberately designed that way. For instance, certain treatment combinations may be more expensive or more difficult to run than others, so fewer observations may be taken in those cells. Alternatively, some treatment combinations may be of greater interest to the experimenter because they represent new or unexplored conditions, so may elect to obtain additional replication in those cells.

The orthogonality property of main effects and interactions present in balanced data does not carry over to the unbalanced case. This means that the usual analysis of variance techniques do not apply. Consequently, the analysis of unbalanced factorials is much more difficult than that for balanced designs.

In this section we give a brief overview of methods for dealing with unbalanced factorials, concentrating on the case of the two-factor fixed effects model. Suppose that the number of observations in the ijth cell is n_{ij}. Furthermore, let $n_{i.} = \sum_{j=1}^{b} n_{ij}$ be the number of observations in the ith row (the ith level of factor A), $n_{.j} = \sum_{i=1}^{a} n_{ij}$ be the number of observations in the jth column (the jth level of factor B), and $n_{..} = \sum_{i=1}^{a} \sum_{j=1}^{b} n_{ij}$ be the total number of observations.

14-2.1 Proportional Data: An Easy Case

One situation involving unbalanced data presents little difficulty in analysis; this is the case of **proportional data**. That is, the number of observations in the ijth cell is

$$n_{ij} = \frac{n_{i.}n_{.j}}{n_{..}} \tag{14-11}$$

This condition implies that the number of observations in any two rows or columns are proportional. When proportional data occur, the standard analysis of variance can be

employed. Only minor modifications are required in the manual computing formulas for the sums of squares, which become

$$SS_T = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n_{ij}} y_{ijk}^2 - \frac{y_{...}^2}{n_{..}}$$

$$SS_A = \sum_{i=1}^{a}\frac{y_{i..}^2}{n_{i.}} - \frac{y_{...}^2}{n_{..}}$$

$$SS_B = \sum_{j=1}^{b}\frac{y_{.j.}^2}{n_{.j}} - \frac{y_{...}^2}{n_{..}}$$

$$SS_{AB} = \sum_{i=1}^{a}\sum_{j=1}^{b}\frac{y_{ij.}^2}{n_{ij}} - \frac{y_{...}^2}{n_{..}} - SS_A - SS_B$$

$$SS_E = SS_T - SS_A - SS_B - SS_{AB}$$

$$= \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n_{ij}} y_{ijk}^2 - \sum_{i=1}^{a}\sum_{j=1}^{b}\frac{y_{ij.}^2}{n_{ij}}$$

As an example of proportional data, consider the battery design experiment in Example 5-1. A modified version of the original data is shown in Table 14-4. Clearly, the data are proportional; for example, in cell 1,1 we have

$$n_{11} = \frac{n_{1.}n_{.1}}{n_{..}} = \frac{10(8)}{20} = 4$$

observations. The results of applying the usual analysis of variance to these data are shown in Table 14-5 on the next page. Both material type and temperature are significant, which agrees with the analysis of the full data set in Example 5-1. However, the interaction noted in Example 5-1 is not present.

14-2.2 Approximate Methods

When unbalanced data are not too far from the balanced case, it is sometimes possible to use **approximate procedures** that convert the unbalanced problem into a balanced

Table 14-4 Battery Design Experiment with Proportional Data

Material Type	Temperature, °F: 15		70		125		
1	$n_{11} = 4$		$n_{12} = 4$		$n_{13} = 2$		$n_{1.} = 10$
	130	155	34	40			
	74	180	80	75	70	58	$y_{1..} = 896$
2	$n_{21} = 2$		$n_{22} = 2$		$n_{23} = 1$		$n_{2.} = 5$
	159	126	136	115	45		$y_{2..} = 581$
3	$n_{31} = 2$		$n_{32} = 2$		$n_{33} = 1$		$n_{3.} = 5$
	138	160	150	139	96		$y_{3..} = 683$
	$n_{.1} = 8$		$n_{.2} = 8$		$n_{.3} = 4$		$n_{..} = 20$
	$y_{.1.} = 1122$		$y_{.2.} = 769$		$y_{.3.} = 269$		$y_{...} = 2160$

Table 14-5 Analysis of Variance for Battery Design Data in Table 14-4

Source of Variance	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Material types	8,170.400	2	4,085.20	5.00
Temperature	16,090.875	2	8,045.44	9.85
Interaction	5,907.725	4	1,476.93	1.18
Error	8,981.000	11	816.45	
Total	39,150.000	19		

one. This of course makes the analysis only approximate, but the analysis of balanced data is so easy that we are frequently tempted to use this approach. In practice, we must decide when the data are not sufficiently different from the balanced case to make the degree of approximation introduced relatively unimportant. We now briefly describe some of these approximate methods. We assume that every cell has at least one observation (i.e., $n_{ij} \geq 1$).

Estimating Missing Observations

If only a few n_{ij} are different, a reasonable procedure is to estimate the missing values. For example, consider the unbalanced design in Table 14-6. Clearly, estimating the single missing value in cell 2,2 is a reasonable approach. For a model with interaction, the estimate of the missing value in the ijth cell that minimizes the error sum of squares is $\bar{y}_{ij}$. That is, we estimate the missing value by taking the average of the observations that are available in that cell.

The estimated value is treated just like actual data. The only modification to the analysis of variance is to reduce the error degrees of freedom by the number of missing observations that have been estimated. For example, if we estimate the missing value in cell 2,2 in Table 14-6, we would use 26 error degrees of freedom instead of 27.

Setting Data Aside

Consider the data in Table 14-7 on the facing page. Note that cell 2,2 has only one more observation than the others. Estimating missing values for the remaining eight cells is probably not a good idea here because this would result in estimates constituting about 18 percent of the final data. An alternative is to set aside one of the observations in cell 2,2, giving a balanced design with $n = 4$ replicates.

The observation that is set aside should be chosen randomly. Furthermore, rather than completely discarding the observation, we could return it to the design, then randomly choose another observation to set aside and repeat the analysis. And, we hope,

Table 14-6 The n_{ij} Values for an Unbalanced Design

	Columns		
Rows	1	2	3
1	4	4	4
2	4	3	4
3	4	4	4

Table 14-7 The n_{ij} Values for an Unbalanced Design

	Columns		
Rows	1	2	3
1	4	4	4
2	4	5	4
3	4	4	4

these two analyses will not lead to conflicting interpretations of the data. If they do, we suspect that the observation that was set aside is an outlier or a wild value and should be handled accordingly. In practice, this confusion is unlikely to occur when only small numbers of observations are set aside and the variability within the cells is small.

Method of Unweighted Means

In this approach, introduced by Yates (1934), the cell averages are treated as data and are subjected to a standard balanced data analysis to obtain sums of squares for rows, columns, and interaction. The error mean square is found as

$$MS_E = \frac{\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij.})^2}{n_{..} - ab} \tag{14-12}$$

Now MS_E estimates σ^2, the variance of y_{ijk}, an individual observation. However, we have done an analysis of variance on the cell *averages*, and because the variance of the average in the ijth cell is σ^2/n_{ij}, the error mean square actually used in the analysis of variance should be an estimate of the average variance of the $\bar{y}_{ij.}$, say

$$\bar{V}(\bar{y}_{ij.}) = \frac{\sum_{i=1}^{a}\sum_{j=1}^{b} \sigma^2/n_{ij}}{ab} = \frac{\sigma^2}{ab}\sum_{i=1}^{a}\sum_{j=1}^{b}\frac{1}{n_{ij}} \tag{14-13}$$

Using MS_E from Equation 14-12 to estimate σ^2 in Equation 14-13, we obtain

$$MS_E' = \frac{MS_E}{ab}\sum_{i=1}^{a}\sum_{j=1}^{b}\frac{1}{n_{ij}} \tag{14-14}$$

as the error mean square (with $n_{..} - ab$ degrees of freedom) to use in the analysis of variance.

The method of unweighted means is an approximate procedure because the sums of squares for rows, columns, and interaction are not distributed as chi-square random variables. The primary advantage of the method seems to be its computational simplicity. When the n_{ij} are not dramatically different, the method of unweighted means often works reasonably well.

A related technique is the **weighted squares of means method**, also proposed by Yates (1934). This technique is also based on the sums of squares of the cell means, but the terms in the sums of squares are weighted in inverse proportion to their variances. For further details of the procedure, see Searle (1971a) and Speed, Hocking, and Hackney (1978).

14-2.3 The Exact Method

In situations where approximate methods are inappropriate, such as when empty cells occur (some $n_{ij} = 0$) or when the n_{ij} are dramatically different, the experimenter must use an exact analysis. The approach used to develop sums of squares for testing main effects and interactions is to represent the analysis of variance model as a **regression model**, fit that model to the data, and use the general regression significance test approach. However, there are several ways that this may be done, and these methods may result in different values for the sums of squares. Furthermore, the hypotheses that are being tested are not always direct analogs of those for the balanced case, nor are they always easily interpretable. For further reading on the subject, see the supplemental text material for this chapter. Other good references are Searle (1971a); Speed and Hocking (1976); Hocking and Speed (1975); Hocking, Hackney, and Speed (1978); Speed, Hocking, and Hackney (1978); Searle, Speed, and Henderson (1981); Searle (1987); and Milliken and Johnson (1984). The SAS system of statistical software provides an excellent approach to the analysis of unbalanced data through PROC GLM.

14-3 THE ANALYSIS OF COVARIANCE

In Chapters 2 and 4 we introduced the use of the blocking principle to improve the precision with which comparisons between treatments are made. The paired t test was the procedure illustrated in Chapter 2 and the randomized block design was presented in Chapter 4. In general, the **blocking principle** can be used to eliminate the effect of controllable nuisance factors. The **analysis of covariance** is another technique that is occasionally useful for improving the precision of an experiment. Suppose that in an experiment with a response variable y there is another variable, say x, and that y is linearly related to x. Furthermore, suppose that x cannot be controlled by the experimenter but can be observed along with y. The variable x is called a **covariate** or **concomitant variable**. The analysis of covariance involves adjusting the observed response variable for the effect of the concomitant variable. If such an adjustment is not performed, the concomitant variable could inflate the error mean square and make true differences in the response due to treatments harder to detect. Thus, the analysis of covariance is a method of adjusting for the effects of an uncontrollable nuisance variable. As we will see, the procedure is a combination of analysis of variance and regression analysis.

As an example of an experiment in which the analysis of covariance may be em-

Table 14-8 Breaking Strength Data (y = strength in pounds and x = diameter in 10^{-3} inches)

Machine 1		Machine 2		Machine 3	
y	x	y	x	y	x
36	20	40	22	35	21
41	25	48	28	37	23
39	24	39	22	42	26
42	25	45	30	34	21
49	32	44	28	32	15
207	126	216	130	180	106

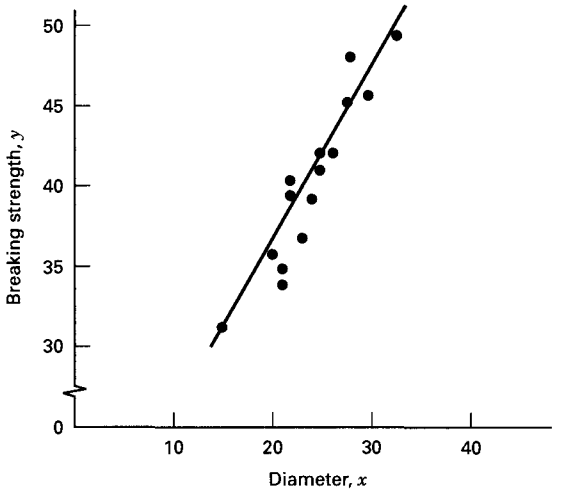


Figure 14-3 Breaking strength (y) versus fiber diameter (x).

ployed, consider a study performed to determine if there is a difference in the strength of a monofilament fiber produced by three different machines. The data from this experiment are shown in Table 14-8 (page 604). Figure 14-3 presents a scatter diagram of strength (y) versus the diameter (or thickness) of the sample. Clearly the strength of the fiber is also affected by its thickness; consequently, a thicker fiber will generally be stronger than a thinner one. The analysis of covariance could be used to remove the effect of thickness (x) on strength (y) when testing for differences in strength between machines.

14-3.1 Description of the Procedure

The basic procedure for the analysis of covariance is now described and illustrated for a single-factor experiment with one covariate. Assuming that there is a linear relationship between the response and the covariate, an appropriate statistical model is

$$y_{ij} = \mu + \tau_i + \beta(x_{ij} - \bar{x}_{..}) + \epsilon_{ij} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, n \end{cases} \tag{14-15}$$

where y_{ij} is the jth observation on the response variable taken under the ith treatment or level of the single factor, x_{ij} is the measurement made on the covariate or concomitant variable corresponding to y_{ij} (i.e., the ijth run), $\bar{x}_{..}$ is the mean of the x_{ij} values, μ is an overall mean, τ_i is the effect of the ith treatment, β is a linear regression coefficient indicating the dependency of y_{ij} on x_{ij}, and ϵ_{ij} is a random error component. We assume that the errors ϵ_{ij} are NID(0, σ^2), that the slope $\beta \neq 0$ and the true relationship between y_{ij} and x_{ij} is linear, that the regression coefficients for each treatment are identical, that the treatment effects sum to zero ($\sum_{i=1}^{a} \tau_i = 0$), and that the concomitant variable x_{ij} is not affected by the treatments.

Notice from Equation 14-15 that the analysis of covariance model is a combination of the linear models employed in analysis of variance and regression. That is, we have treatment effects $\{\tau_i\}$ as in a single-factor analysis of variance and a regression coefficient β as in a regression equation. The concomitant variable in Equation 14-15 is expressed

as $(x_{ij} - \bar{x}_{..})$ instead of x_{ij} so that the parameter μ is preserved as the overall mean. The model could have been written as

$$y_{ij} = \mu' + \tau_i + \beta x_{ij} + \epsilon_{ij} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, n \end{cases} \tag{14-16}$$

where μ' is a constant not equal to the overall mean, which for this model is $\mu' + \beta\bar{x}_{..}$. Equation 14-15 is more widely found in the literature.

To describe the analysis, we introduce the following notation:

$$S_{yy} = \sum_{i=1}^{a}\sum_{j=1}^{n}(y_{ij} - \bar{y}_{..})^2 = \sum_{i=1}^{a}\sum_{j=1}^{n} y_{ij}^2 - \frac{y_{..}^2}{an} \tag{14-17}$$

$$S_{xx} = \sum_{i=1}^{a}\sum_{j=1}^{n}(x_{ij} - \bar{x}_{..})^2 = \sum_{i=1}^{a}\sum_{j=1}^{n} x_{ij}^2 - \frac{x_{..}^2}{an} \tag{14-18}$$

$$S_{xy} = \sum_{i=1}^{a}\sum_{j=1}^{n}(x_{ij} - \bar{x}_{..})(y_{ij} - \bar{y}_{..}) = \sum_{i=1}^{a}\sum_{j=1}^{n} x_{ij}y_{ij} - \frac{(x_{..})(y_{..})}{an} \tag{14-19}$$

$$T_{yy} = n\sum_{i=1}^{a}(\bar{y}_{i.} - \bar{y}_{..})^2 = \frac{1}{n}\sum_{i=1}^{a} y_{i.}^2 - \frac{y_{..}^2}{an} \tag{14-20}$$

$$T_{xx} = n\sum_{i=1}^{a}(\bar{x}_{i.} - \bar{x}_{..})^2 = \frac{1}{n}\sum_{i=1}^{a} x_{i.}^2 - \frac{x_{..}^2}{an} \tag{14-21}$$

$$T_{xy} = n\sum_{i=1}^{a}(\bar{x}_{i.} - \bar{x}_{..})(\bar{y}_{i.} - \bar{y}_{..}) = \frac{1}{n}\sum_{i=1}^{a}(x_{i.})(y_{i.}) - \frac{(x_{..})(y_{..})}{an} \tag{14-22}$$

$$E_{yy} = \sum_{i=1}^{a}\sum_{j=1}^{n}(y_{ij} - \bar{y}_{i.})^2 = S_{yy} - T_{yy} \tag{14-23}$$

$$E_{xx} = \sum_{i=1}^{a}\sum_{j=1}^{n}(x_{ij} - \bar{x}_{i.})^2 = S_{xx} - T_{xx} \tag{14-24}$$

$$E_{xy} = \sum_{i=1}^{a}\sum_{j=1}^{n}(x_{ij} - \bar{x}_{i.})(y_{ij} - \bar{y}_{i.}) = S_{xy} - T_{xy} \tag{14-25}$$

Note that, in general, $S = T + E$, where the symbols S, T, and E are used to denote sums of squares and cross-products for total, treatments, and error, respectively. The sums of squares for x and y must be nonnegative; however, the sums of cross-products (xy) may be negative.

We now show how the analysis of covariance adjusts the response variable for the effect of the covariate. Consider the full model (Equation 14-15). The least squares estimators of μ, τ_i, and β are $\hat{\mu} = \bar{y}_{..}$, $\hat{\tau}_i = \bar{y}_{i.} - \bar{y}_{..} - \hat{\beta}(\bar{x}_{i.} - \bar{x}_{..})$, and

$$\hat{\beta} = \frac{E_{xy}}{E_{xx}} \tag{14-26}$$

The error sum of squares in this model is

$$SS_E = E_{yy} - (E_{xy})^2/E_{xx} \tag{14-27}$$

with $a(n - 1) - 1$ degrees of freedom. The experimental error variance is estimated by

$$MS_E = \frac{SS_E}{a(n - 1) - 1}$$

Now suppose that there is no treatment effect. The model (Equation 14-15) would then be

$$y_{ij} = \mu + \beta(x_{ij} - \bar{x}_{..}) + \epsilon_{ij} \tag{14-28}$$

and it can be shown that the least squares estimators of μ and β are $\hat{\mu} = \bar{y}_{..}$ and $\hat{\beta} = S_{xy}/S_{xx}$. The sum of squares for error in this reduced model is

$$SS'_E = S_{yy} - (S_{xy})^2/S_{xx} \tag{14-29}$$

with $an - 2$ degrees of freedom. In Equation 14-29, the quantity $(S_{xy})^2/S_{xx}$ is the reduction in the sum of squares of y obtained through the linear regression of y on x. Furthermore, note that SS_E is smaller than SS'_E [because the model (Equation 14-15) contains additional parameters $\{\tau_i\}$] and that the quantity $SS'_E - SS_E$ is a reduction in sum of squares due to the $\{\tau_i\}$. Therefore, the difference between SS'_E and SS_E, that is, $SS'_E - SS_E$, provides a sum of squares with $a - 1$ degrees of freedom for testing the hypothesis of no treatment effects. Consequently, to test $H_0: \tau_i = 0$, compute

$$F_0 = \frac{(SS'_E - SS_E)/(a - 1)}{SS_E/[a(n - 1) - 1]} \tag{14-30}$$

which, if the null hypothesis is true, is distributed as $F_{a-1,a(n-1)-1}$. Thus, we reject $H_0: \tau_i = 0$ if $F_0 > F_{\alpha,a-1,a(n-1)-1}$. The P value approach could also be used.

It is instructive to examine the display in Table 14-9 on the next page. In this table we have presented the analysis of covariance as an "adjusted" analysis of variance. In the source of variation column, the total variability is measured by S_{yy} with $an - 1$ degrees of freedom. The source of variation "regression" has the sum of squares $(S_{xy})^2/S_{xx}$ with one degree of freedom. If there were no concomitant variable, we would have $S_{xy} = S_{xx} = E_{xy} = E_{xx} = 0$. Then the sum of squares for error would be simply E_{yy} and the sum of squares for treatments would be $S_{yy} - E_{yy} = T_{yy}$. However, because of the presence of the concomitant variable, we must "adjust" S_{yy} and E_{yy} for the regression of y on x as shown in Table 14-9. The adjusted error sum of squares has $a(n - 1) - 1$ degrees of freedom instead of $a(n - 1)$ degrees of freedom because an additional parameter (the slope β) is fitted to the data.

The computations are usually displayed in an analysis of covariance table such as Table 14-10 on the next page. This layout is employed because it conveniently summarizes all the required sums of squares and cross-products as well as the sums of squares for testing hypotheses about treatment effects. In addition to testing the hypothesis that there are no differences in the treatment effects, we frequently find it useful in interpreting the data to present the adjusted treatment means. These adjusted means are computed according to

$$\text{Adjusted } \bar{y}_{i.} = \bar{y}_{i.} - \hat{\beta}(\bar{x}_{i.} - \bar{x}_{..}) \qquad i = 1, 2, \ldots, a \tag{14-31}$$

where $\hat{\beta} = E_{xy}/E_{xx}$. This adjusted treatment mean is the least squares estimator of $\mu + \tau_i$, $i = 1, 2, \ldots, a$, in the model (Equation 14-15). The standard error of any adjusted treatment mean is

$$S_{\text{adj}\bar{y}_{i.}} = \left[MS_E \left(\frac{1}{n} + \frac{(\bar{x}_{i.} - \bar{x}_{..})^2}{E_{xx}} \right) \right]^{1/2} \tag{14-32}$$

Table 14-9 Analysis of Covariance as an "Adjusted" Analysis of Variance

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Regression	$(S_{xy})^2/S_{xx}$	1		
Treatments	$SS'_E - SS_E = S_{yy} - (S_{xy})^2/S_{xx} - [E_{yy} - (E_{xy})^2/E_{xx}]$	$a - 1$	$\dfrac{SS'_E - SS_E}{a - 1}$	$\dfrac{(SS'_E - SS_E)/(a - 1)}{MS_E}$
Error	$SS_E = E_{yy} - (E_{xy})^2/E_{xx}$	$a(n - 1) - 1$	$MS_E = \dfrac{SS_E}{a(n - 1) - 1}$	
Total	S_{yy}	$an - 1$		

Table 14-10 Analysis of Covariance for a Single-Factor Experiment with One Covariate

		Sums of Squares and Products			Adjusted for Regression		
Source of Variation	Degrees of Freedom	x	xy	y	y	Degrees of Freedom	Mean Square
Treatments	$a - 1$	T_{xx}	T_{xy}	T_{yy}			
Error	$a(n - 1)$	E_{xx}	E_{xy}	E_{yy}	$SS_E = E_{yy} - (E_{xy})^2/E_{xx}$	$a(n - 1) - 1$	$MS_E = \dfrac{SS_E}{a(n - 1) - 1}$
Total	$an - 1$	S_{xx}	S_{xy}	S_{yy}	$SS'_E = S_{yy} - (S_{xy})^2/S_{xx}$	$an - 2$	
Adjusted Treatments					$SS'_E - SS_E$	$a - 1$	$\dfrac{SS'_E - SS_E}{a - 1}$

Finally, we recall that the regression coefficient β in the model (Equation 14-15) has been assumed to be nonzero. We may test the hypothesis $H_0: \beta = 0$ by using the test statistic

$$F_0 = \frac{(E_{xy})^2/E_{xx}}{MS_E} \tag{14-33}$$

which under the null hypothesis is distributed as $F_{1,a(n-1)-1}$. Thus, we reject $H_0: \beta = 0$ if $F_0 > F_{\alpha,1,a(n-1)-1}$.

EXAMPLE 14-4

Consider the experiment described at the beginning of Section 14-3. Three different machines produce a monofilament fiber for a textile company. The process engineer is interested in determining if there is a difference in the breaking strength of the fiber produced by the three machines. However, the strength of a fiber is related to its diameter, with thicker fibers being generally stronger than thinner ones. A random sample of five fiber specimens is selected from each machine. The fiber strength (y) and the corresponding diameter (x) for each specimen are shown in Table 14-8.

The scatter diagram of breaking strength versus the fiber diameter (Figure 14-3) shows a strong suggestion of a linear relationship between breaking strength and diameter, and it seems appropriate to remove the effect of diameter on strength by an analysis of covariance. Assuming that a linear relationship between breaking strength and diameter is appropriate, the model is

$$y_{ij} = \mu + \tau_i + \beta(x_{ij} - \bar{x}_{..}) + \epsilon_{ij} \qquad \begin{cases} i = 1, 2, 3 \\ j = 1, 2, \ldots, 5 \end{cases}$$

Using Equations 14-17 through 14-25, we may compute

$$S_{yy} = \sum_{i=1}^{3}\sum_{j=1}^{5} y_{ij}^2 - \frac{y_{..}^2}{an} = (36)^2 + (41)^2 + \cdots + (32)^2 - \frac{(603)^2}{(3)(5)} = 346.40$$

$$S_{xx} = \sum_{i=1}^{3}\sum_{j=1}^{5} x_{ij}^2 - \frac{x_{..}^2}{an} = (20)^2 + (25)^2 + \cdots + (15)^2 - \frac{(362)^2}{(3)(5)} = 261.73$$

$$S_{xy} = \sum_{i=1}^{3}\sum_{j=1}^{5} x_{ij}y_{ij} - \frac{(x_{..})(y_{..})}{an} = (20)(36) + (25)(41) + \cdots + (15)(32) - \frac{(362)(603)}{(3)(5)} = 282.60$$

$$T_{yy} = \frac{1}{n}\sum_{i=1}^{3} y_{i.}^2 - \frac{y_{..}^2}{an} = \frac{1}{5}[(207)^2 + (216)^2 + (180)^2] - \frac{(603)^2}{(3)(5)} = 140.40$$

$$T_{xx} = \frac{1}{n}\sum_{i=1}^{3} x_{i.}^2 - \frac{x_{..}^2}{an} = \frac{1}{5}[(126)^2 + (130)^2 + (106)^2] - \frac{(362)^2}{(3)(5)} = 66.13$$

$$T_{xy} = \frac{1}{n}\sum_{i=1}^{3} x_{i.}y_{i.} - \frac{(x_{..})(y_{..})}{an} = \frac{1}{5}[(126)(207) + (130)(216) + (106)(184)] - \frac{(362)(603)}{(3)(5)} = 96.00$$

$$E_{yy} = S_{yy} - T_{yy} = 346.40 - 140.40 = 206.00$$
$$E_{xx} = S_{xx} - T_{xx} = 261.73 - 66.13 = 195.60$$
$$E_{xy} = S_{xy} - T_{xy} = 282.60 - 96.00 = 186.60$$

From Equation 14-29, we find

$$\begin{aligned} SS'_E &= S_{yy} - (S_{xy})^2/S_{xx} \\ &= 346.40 - (282.60)^2/261.73 \\ &= 41.27 \end{aligned}$$

with $an - 2 = (3)(5) - 2 = 13$ degrees of freedom; and from Equation 14-27, we find

$$\begin{aligned} SS_E &= E_{yy} - (E_{xy})^2/E_{xx} \\ &= 206.00 - (186.60)^2/195.60 \\ &= 27.99 \end{aligned}$$

with $a(n - 1) - 1 = 3(5 - 1) - 1 = 11$ degrees of freedom.

The sum of squares for testing $H_0: \tau_1 = \tau_2 = \tau_3 = 0$ is

$$\begin{aligned} SS'_E - SS_E &= 41.27 - 27.99 \\ &= 13.28 \end{aligned}$$

with $a - 1 = 3 - 1 = 2$ degrees of freedom. These calculations are summarized in Table 14–11 on the next page.

To test the hypothesis that machines differ in the breaking strength of fiber produced, that is, $H_0: \tau_i = 0$, we compute the test statistic from Equation 14-30 as

$$\begin{aligned} F_0 &= \frac{(SS'_E - SS_E)/(a - 1)}{SS_E/[a(n - 1) - 1]} \\ &= \frac{13.28/2}{27.99/11} = \frac{6.64}{2.54} = 2.61 \end{aligned}$$

Comparing this to $F_{0.10,2,11} = 2.86$, we find that the null hypothesis cannot be rejected. The P value of this test statistic is $P = 0.1181$. Thus there is no strong evidence that the fibers produced by the three machines differ in breaking strength.

The estimate of the regression coefficient is computed from Equation 14-26 as

$$\hat{\beta} = \frac{E_{xy}}{E_{xx}} = \frac{186.60}{195.60} = 0.9540$$

We may test the hypothesis $H_0: \beta = 0$ by using Equation 14-33. The test statistic is

$$F_0 = \frac{(E_{xy})^2/E_{xx}}{MS_E} = \frac{(186.60)^2/195.60}{2.54} = 70.08$$

and because $F_{0.01,1,11} = 9.65$, we reject the hypothesis that $\beta = 0$. Therefore, there is a linear relationship between breaking strength and diameter, and the adjustment provided by the analysis of covariance was necessary.

Table 14-11 Analysis of Covariance for the Breaking Strength Data

Source of Variation	Degrees of Freedom	Sums of Squares and Products			Adjusted for Regression				
		x	xy	y	y	Degrees of Freedom	Mean Square	F_0	P Value
Machines	2	66.13	96.00	140.40					
Error	12	195.60	186.60	206.00	27.99	11	2.54		
Total	14	261.73	282.60	346.40	41.27	13			
Adjusted Machines					13.28	2	6.64	2.61	0.1181

The adjusted treatment means may be computed from Equation 14-31. These adjusted means are

$$\begin{aligned}\text{Adjusted } \bar{y}_{1.} &= \bar{y}_{1.} - \hat{\beta}(\bar{x}_{1.} - \bar{x}_{..}) \\ &= 41.40 - (0.9540)(25.20 - 24.13) = 40.38 \\ \text{Adjusted } \bar{y}_{2.} &= \bar{y}_{2.} - \hat{\beta}(\bar{x}_{2.} - \bar{x}_{..}) \\ &= 43.20 - (0.9540)(26.00 - 24.13) = 41.42\end{aligned}$$

and

$$\begin{aligned}\text{Adjusted } \bar{y}_{3.} &= \bar{y}_{3.} - \hat{\beta}(\bar{x}_{3.} - \bar{x}_{..}) \\ &= 36.00 - (0.9540)(21.20 - 24.13) = 38.80\end{aligned}$$

Comparing the adjusted treatment means with the unadjusted treatment means (the $\bar{y}_{i.}$), we note that the adjusted means are much closer together, another indication that the covariance analysis was necessary.

A basic assumption in the analysis of covariance is that the treatments do not influence the covariate x because the technique removes the effect of variations in the $\bar{x}_{i.}$. However, if the variability in the $\bar{x}_{i.}$ is due in part to the treatments, then analysis of covariance removes part of the treatment effect. Thus, we must be reasonably sure that the treatments do not affect the values x_{ij}. In some experiments this may be obvious from the nature of the covariate, whereas in others it may be more doubtful. In our example, there may be a difference in fiber diameter (x_{ij}) between the three machines. In such cases, Cochran and Cox (1957) suggest that an analysis of variance on the x_{ij} values may be helpful in determining the validity of this assumption. For our problem, this procedure yields

$$F_0 = \frac{66.13/2}{195.60/12} = \frac{33.07}{16.30} = 2.03$$

which is less than $F_{0.10,2,12} = 2.81$, so there is no reason to believe that machines produce fibers of different diameters.

Diagnostic checking of the covariance model is based on residual analysis. For the covariance model, the residuals are

$$e_{ij} = y_{ij} - \hat{y}_{ij}$$

where the fitted values are

$$\begin{aligned}\hat{y}_{ij} &= \hat{\mu} + \hat{\tau}_i + \hat{\beta}(x_{ij} - \bar{x}_{..}) = \bar{y}_{..} + [\bar{y}_{i.} - \bar{y}_{..} - \hat{\beta}(\bar{x}_{i.} - \bar{x}_{..})] \\ &\quad + \hat{\beta}(x_{ij} - \bar{x}_{..}) = \bar{y}_{i.} + \hat{\beta}(x_{ij} - \bar{x}_{i.})\end{aligned}$$

Thus,

$$e_{ij} = y_{ij} - \bar{y}_{i.} - \hat{\beta}(x_{ij} - \bar{x}_{i.}) \tag{14-34}$$

To illustrate the use of Equation 14-34, the residual for the first observation from the first machine in Example 14-4 is

$$\begin{aligned}e_{11} &= y_{11} - \bar{y}_{1.} - \hat{\beta}(x_{11} - \bar{x}_{1.}) = 36 - 41.4 - (0.9540)(20 - 25.2) \\ &= 36 - 36.4392 = -0.4392\end{aligned}$$

A complete listing of observations, fitted values, and residuals is given in the following table:

Observed Value y_{ij}	Fitted Value $\hat{y}_{ij}$	Residual $e_{ij} = y_{ij} - \hat{y}_{ij}$
36	36.4392	−0.4392
41	41.2092	−0.2092
39	40.2552	−1.2552
42	41.2092	0.7908
49	47.8871	1.1129
40	39.3840	0.6160
48	45.1079	2.8921
39	39.3840	−0.3840
45	47.0159	−2.0159
44	45.1079	−1.1079
35	35.8092	−0.8092
37	37.7171	−0.7171
42	40.5791	1.4209
34	35.8092	−1.8092
32	30.0852	1.9148

The residuals are plotted versus the fitted values $\hat{y}_{ij}$ in Figure 14-4, versus the covariate x_{ij} in Figure 14-5 (page 614) and versus the machines in Figure 14-6 (page 614). A normal probability plot of the residuals is shown in Figure 14-7 (page 615). These plots do not reveal any major departures from the assumptions, so we conclude that the covariance model (Equation 14-15) is appropriate for the breaking strength data.

It is interesting to note what would have happened in this experiment if an analysis of covariance had not been performed, that is, if the breaking strength data (y) had been analyzed as a single-factor experiment in which the covariate x was ignored. The analysis of variance of the breaking strength data is shown in Table 14-12 (page 615). We would conclude, based on this analysis, that machines differ significantly in the strength of fiber

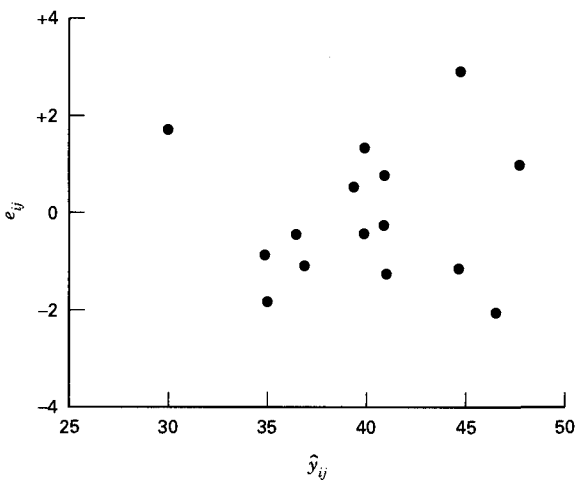


Figure 14-4 Plot of residuals versus fitted values for Example 14-4.

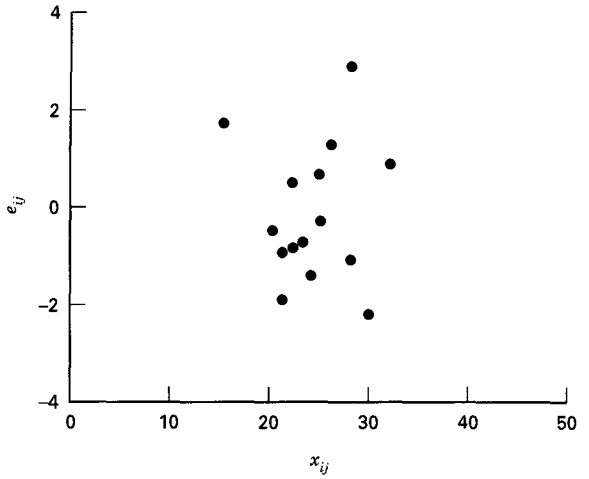


Figure 14-5 Plot of residuals versus fiber diameter x for Example 14-4.

produced. This is exactly *opposite the conclusion* reached by the covariance analysis. If we suspected that the machines differed significantly in their effect on fiber strength, then we would try to equalize the strength output of the three machines. However, in this problem the machines do not differ in the strength of fiber produced after the linear effect of fiber diameter is removed. It would be helpful to reduce the within-machine fiber diameter variability because this would probably reduce the strength variability in the fiber.

14-3.2 Computer Solution

There are several computer software packages available that can perform the analysis of covariance. The output from the Minitab General Linear Models procedure for the data

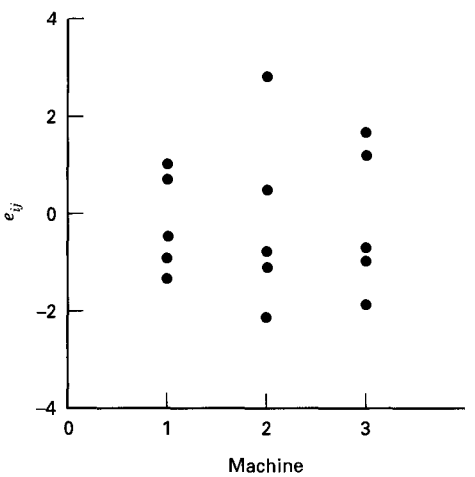


Figure 14-6 Plot of residuals versus machine.

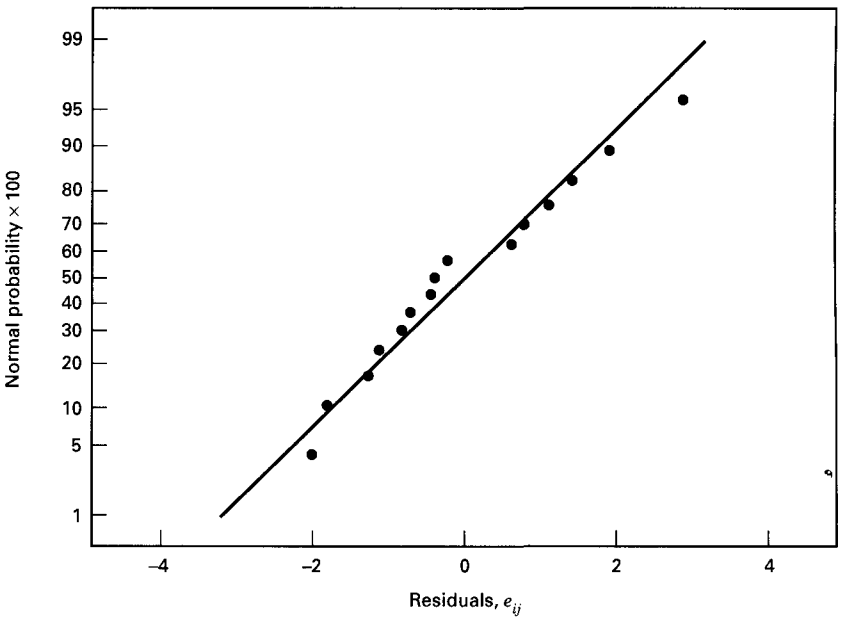


Figure 14-7 Normal probability plot of residuals from Example 14-4.

in Example 14-4 is shown in Table 14-13 (on the following page). This output is very similar to those presented previously. In the section of the output entitled "Analysis of Variance," the "Seq SS" correspond to a "sequential" partitioning of the overall model sum of squares, say

$$\begin{aligned} SS\ (\text{Model}) &= SS\ (\text{Diameter}) + SS\ (\text{Machine}\,|\,\text{Diameter}) \\ &= 305.13 + 13.28 \\ &= 318.41 \end{aligned}$$

whereas the "Adj SS" corresponds to the "extra" sum of squares for each factor, that is,

$$SS\ (\text{Machine}\,|\,\text{Diameter}) = 13.28$$

and

$$SS\ (\text{Diameter}\,|\,\text{Machine}) = 178.01$$

Note that SS (Machine | Diameter) is the correct sum of squares to use for testing for no machine effect, and SS (Diameter | Machine) is the correct sum of squares to use for testing the hypothesis that $\beta = 0$. The test statistics in Table 14-13 differ slightly from those computed manually because of rounding.

Table 14-12 Incorrect Analysis of the Breaking Strength Data as a Single-Factor Experiment

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P Value
Machines	140.40	2	70.20	4.09	0.0442
Error	206.00	12	17.17		
Total	346.40	14			

Table 14-13 Minitab Output (Analysis of Covariance) for Example 14-4

General Linear Model

```
Factor      Type Levels Values
Machine    fixed      3 1 2 3

Analysis of Variance for Strength, using Adjusted SS for Tests

Source      DF      Seq SS      Adj SS      Adj MS        F       P
Diameter     1      305.13      178.01      178.01    69.97   0.000
Machine      2       13.28       13.28        6.64     2.61   0.118
Error       11       27.99       27.99        2.54
Total       14      346.40

Term            Coef      StDev         T       P
Constant      17.177      2.783      6.17   0.000
Diameter      0.9540     0.1140      8.36   0.000
Machine
1             0.1824     0.5950      0.31   0.765
2             1.2192     0.6201      1.97   0.075

Means for Covariates

Covariate       Mean      StDev
Diameter       24.13      4.324

Least Squares Means for Strength

Machine       Mean      StDev
1            40.38     0.7236
2            41.42     0.7444
3            38.80     0.7879
```

The program also computes the adjusted treatment means from Equation 14-31 (Minitab refers to those as least squares means on the sample output) and the standard errors. The program will also compare all pairs of treatment means using the pairwise multiple comparison procedures discussed in Chapter 3.

14-3.3 Development by the General Regression Significance Test

It is possible to develop formally the procedure for testing $H_0: \tau_i = 0$ in the covariance model

$$y_{ij} = \mu + \tau_i + \beta(x_{ij} - \bar{x}_{..}) + \epsilon_{ij} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, n \end{cases} \tag{14-35}$$

using the general regression significance test. Consider estimating the parameters in the model (Equation 14-15) by least squares. The least squares function is

$$L = \sum_{i=1}^{a} \sum_{j=1}^{n} [y_{ij} - \mu - \tau_i - \beta(x_{ij} - \bar{x}_{..})]^2 \tag{14-36}$$

and from $\partial L/\partial\mu = \partial L/\partial\tau_i = \partial L/\partial\beta = 0$, we obtain the normal equations

$$\mu: an\hat{\mu} + n\sum_{i=1}^{a}\hat{\tau}_i = y_{..} \tag{14-37a}$$

$$\tau_i: n\hat{\mu} + n\hat{\tau}_i + \hat{\beta}\sum_{j=1}^{n}(x_{ij} - \bar{x}_{..}) = y_{i.} \qquad i = 1, 2, \ldots, a \tag{14-37b}$$

$$\beta: \sum_{i=1}^{a}\hat{\tau}_i\sum_{j=1}^{n}(x_{ij} - \bar{x}_{..}) + \hat{\beta}S_{xx} = S_{xy} \tag{14-37c}$$

Adding the a equations in Equation 14-37b, we obtain Equation 14-37a because $\Sigma_{i=1}^{a}\Sigma_{j=1}^{n}(x_{ij} - \bar{x}_{..}) = 0$, so there is one linear dependency in the normal equations. Therefore, it is necessary to augment Equations 14-37 with a linearly independent equation to obtain a solution. A logical side condition is $\Sigma_{i=1}^{a}\hat{\tau}_i = 0$.

Using this condition, we obtain from Equation 14-37a

$$\hat{\mu} = \bar{y}_{..} \tag{14-38a}$$

and from Equation 14-37b

$$\hat{\tau}_i = \bar{y}_{i.} - \bar{y}_{..} - \hat{\beta}(\bar{x}_{i.} - \bar{x}_{..}) \tag{14-38b}$$

Equation 14-37c may be rewritten as

$$\sum_{i=1}^{a}(\bar{y}_{i.} - \bar{y}_{..})\sum_{j=1}^{n}(x_{ij} - \bar{x}_{..}) - \hat{\beta}\sum_{i=1}^{a}(\bar{x}_{i.} - \bar{x}_{..})\sum_{j=1}^{n}(x_{ij} - \bar{x}_{..}) + \hat{\beta}S_{xx} = S_{xy}$$

after substituting for $\hat{\tau}_i$. But we see that

$$\sum_{i=1}^{a}(\bar{y}_{i.} - \bar{y}_{..})\sum_{j=1}^{n}(x_{ij} - \bar{x}_{..}) = T_{xy}$$

and

$$\sum_{i=1}^{a}(\bar{x}_{i.} - \bar{x}_{..})\sum_{j=1}^{n}(x_{ij} - \bar{x}_{..}) = T_{xx}$$

Therefore, the solution to Equation 14-37c is

$$\hat{\beta} = \frac{S_{xy} - T_{xy}}{S_{xx} - T_{xx}} = \frac{E_{xy}}{E_{xx}}$$

which was the result given previously in Section 14-3.1, Equation 14-26.

We may express the reduction in the total sum of squares due to fitting the model (Equation 14-15) as

$$\begin{aligned}
R(\mu, \tau, \beta) &= \hat{\mu}y_{..} + \sum_{i=1}^{a}\hat{\tau}_i y_{i.} + \hat{\beta}S_{xy} \\
&= (\bar{y}_{..})y_{..} + \sum_{i=1}^{a}[\bar{y}_{i.} - \bar{y}_{..} - (E_{xy}/E_{xx})(\bar{x}_{i.} - \bar{x}_{..})]y_{i.} + (E_{xy}/E_{xx})S_{xy} \\
&= y_{..}^2/an + \sum_{i=1}^{a}(\bar{y}_{i.} - \bar{y}_{..})y_{i.} - (E_{xy}/E_{xx})\sum_{i=1}^{a}(\bar{x}_{i.} - \bar{x}_{..})y_{i.} + (E_{xy}/E_{xx})S_{xy} \\
&= y_{..}^2/an + T_{yy} - (E_{xy}/E_{xx})(T_{xy} - S_{xy}) \\
&= y_{..}^2/an + T_{yy} + (E_{xy})^2/E_{xx}
\end{aligned}$$

This sum of squares has $a + 1$ degrees of freedom because the rank of the normal equations is $a + 1$. The error sum of squares for this model is

$$\begin{aligned} SS_E &= \sum_{i=1}^{a}\sum_{j=1}^{n} y_{ij}^2 - R(\mu, \tau, \beta) \\ &= \sum_{i=1}^{a}\sum_{j=1}^{n} y_{ij}^2 - y_{..}^2/an - T_{yy} - (E_{xy})^2/E_{xx} \\ &= S_{yy} - T_{yy} - (E_{xy})^2/E_{xx} \\ &= E_{yy} - (E_{xy})^2/E_{xx} \end{aligned} \tag{14-39}$$

with $an - (a + 1) = a(n - 1) - 1$ degrees of freedom. This quantity was obtained previously as Equation 14-27.

Now consider the model restricted to the null hypothesis, that is, to $H_0: \tau_1 = \tau_2 = \cdots = \tau_a = 0$. This reduced model is

$$y_{ij} = \mu + \beta(x_{ij} - \bar{x}_{..}) + \epsilon_{ij} \qquad \begin{cases} i = 1, 2, \ldots, a \\ j = 1, 2, \ldots, n \end{cases} \tag{14-40}$$

This is a simple linear regression model, and the least squares normal equations for this model are

$$an\hat{\mu} = y_{..} \tag{14-41a}$$

$$\hat{\beta}S_{xx} = S_{xy} \tag{14-41b}$$

The solutions to these equations are $\hat{\mu} = \bar{y}_{..}$ and $\hat{\beta} = S_{xy}/S_{xx}$, and the reduction in the total sum of squares due to fitting the reduced model is

$$\begin{aligned} R(\mu, \beta) &= \hat{\mu}y_{..} + \hat{\beta}S_{xy} \\ &= (\bar{y}_{..})y_{..} + (S_{xy}/S_{xx})S_{xy} \\ &= y_{..}^2/an + (S_{xy})^2/S_{xx} \end{aligned} \tag{14-42}$$

This sum of squares has two degrees of freedom.

We may find the appropriate sum of squares for testing $H_0: \tau_1 = \tau_2 = \cdots = \tau_a = 0$ as

$$\begin{aligned} R(\tau|\mu, \beta) &= R(\mu, \tau, \beta) - R(\mu, \beta) \\ &= y_{..}^2/an + T_{yy} + (E_{xy})^2/E_{xx} - y_{..}^2/an - (S_{xy})^2/S_{xx} \\ &= S_{yy} - (S_{xy})^2/S_{xx} - [E_{yy} - (E_{xy})^2/E_{xx}] \end{aligned} \tag{14-43}$$

using $T_{yy} = S_{yy} - E_{yy}$. Note that $R(\tau|\mu, \beta)$ has $a + 1 - 2 = a - 1$ degrees of freedom and is identical to the sum of squares given by $SS_E' - SS_E$ in Section 14-3.1. Thus, the test statistic for $H_0: \tau_i = 0$ is

$$F_0 = \frac{R(\tau|\mu, \beta)/(a - 1)}{SS_E/[a(n - 1) - 1]} = \frac{(SS_E' - SS_E)/(a - 1)}{SS_E/[a(n - 1) - 1]} \tag{14-44}$$

which we gave previously as Equation 14-30. Therefore, by using the general regression significance test, we have justified the heuristic development of the analysis of covariance in Section 14-3.1.

14-3.4 Factorial Experiments with Covariates

Analysis of covariance can be applied to more complex treatment structures, such as factorial designs. Provided enough data exists for every treatment combination, nearly any complex treatment structure can be analyzed through the analysis of covariance approach. We now show how the analysis of covariance could be used in the most common family of factorial designs used in industrial experimentation, the 2^k factorials.

Imposing the assumption that the covariate affects the response variable identically across all treatment combinations, an analysis of covariance table similar to the procedure given in Section 14-3.1 could be performed. The only difference would be the treatment sum of squares. For a 2^2 factorial with n replicates, the treatment sum of squares (T_{yy}) would be $(1/n)\ \Sigma_{i=1}^{2}\ \Sigma_{j=1}^{2}\ y_{ij.}^2 - y_{...}^2/(2)(2)n$. This quantity is the sum of the sums of squares for factors A, B, and the AB interaction. The adjusted treatment sum of squares could then be partitioned into individual effect components, that is, adjusted main effects sum of squares SS_A and SS_B, and an adjusted interaction sum of squares, SS_{AB}.

The amount of replication is a key issue when broadening the design structure of the treatments. Consider a 2^3 factorial arrangement. A minimum of two replicates is needed to evaluate all treatment combinations with a separate covariate for each treatment combination (covariate by treatment interaction). This is equivalent to fitting a simple regression model to each treatment combination or design cell. With two observations per cell, one degree of freedom is used to estimate the intercept (the treatment effect), and the other is used to estimate the slope (the covariate effect). With this saturated model, no degrees of freedom are available to estimate the error. Thus, at least three replicates are needed for a complete analysis of covariance, assuming the most general case. This problem becomes more pronounced as the number of distinct design cells (treatment combinations) and covariates increases.

If the amount of replication is limited, various assumptions can be made to allow some useful analysis. The simplest assumption (and typically the worst) that can be made is that the covariate has no effect. If the covariate is erroneously not considered, the entire analysis and subsequent conclusions could be dramatically in error. Another choice is to assume that there is no treatment by covariate interaction. Even if this assumption is incorrect, the average affect of the covariate across all treatments will still increase the precision of the estimation and testing of the treatment effects. One disadvantage of this assumption is that if several treatment levels interact with the covariate, the various terms may cancel one another out and the covariate term, if estimated alone with no interaction, may be insignificant. A third choice would be to assume some of the factors (such as some two-factor and higher interactions) are insignificant. This allows some degrees of freedom to be used to estimate error. This course of action, however, should be undertaken carefully and the subsequent models evaluated thoroughly because the estimation of error will be relatively imprecise unless enough degrees of freedom are allocated for it. With two replicates, each of these assumptions will free some degrees of freedom to estimate error and allow useful hypothesis tests to be performed. Which assumption to enforce should be dictated by the experimental situation and how much risk the experimenter is willing to assume. We caution that in the effects model building strategy if a treatment factor is eliminated, then the resulting two "replicates" of each original 2^3 are not truly replicates. These "hidden replicates" do free degrees of freedom for parameter estimation but should not be used as replicates to estimate pure error because the execution of the original design may not have been randomized that way.

Table 14-14 Response and Covariate Data for a 2^3 with 2 Replicates

A	B	C	x	y
−1	−1	−1	4.05	−30.73
1	−1	−1	0.36	9.07
−1	1	−1	5.03	39.72
1	1	−1	1.96	16.30
−1	−1	1	5.38	−26.39
1	−1	1	8.63	54.58
−1	1	1	4.10	44.54
1	1	1	11.44	66.20
−1	−1	−1	3.58	−26.46
1	−1	−1	1.06	10.94
−1	1	−1	15.53	103.01
1	1	−1	2.92	20.44
−1	−1	1	2.48	−8.94
1	−1	1	13.64	73.72
−1	1	1	−0.67	15.89
1	1	1	5.13	38.57

To illustrate some of these ideas, consider the 2^3 factorial design with two replicates and a covariate shown in Table 14-14. If the response variable y is analyzed without accounting for the covariate, the following model results:

$$\hat{y} = 25.03 + 11.20A + 18.05B + 7.24C - 18.91AB + 14.80AC$$

The overall model is significant at the $\alpha = 0.01$ level with $R^2 = 0.786$ and $MS_E = 470.82$. The residual analysis indicates no problem with this model except the observation with $y = 103.01$ is unusual.

If the second assumption, common slopes with no treatment by covariate interaction, is chosen, the full effects model and the covariate effect can be estimated. The Minitab output (from the General Linear Models routine) is shown in Table 14-15 on the facing page. Notice that the MS_E has been reduced considerably by considering the covariate. The final resulting analysis after sequentially removing each nonsignificant interaction and the main effect C is shown in Table 14-16 on the facing page. This reduced model provides an even smaller MS_E than does the full model with the covariate in Table 14-15.

Finally, we could consider a third course of action, assuming certain interaction terms are negligible. We consider the full model that allows for different slopes between treatments and treatment by covariate interaction. We assume that the three-factor interactions (both ABC and $ABCx$) are not significant and use their associated degrees of freedom to estimate error in the most general effects model that can be fit. This is often a practical assumption. Three-factor and higher interactions are usually negligible in most experimental settings. The current version of Minitab cannot model covariates that interact with treatments, so we use SAS PROC GLM. The type III sums of squares are the adjusted sums of squares that we require. Table 14-17 (page 622) presents the SAS results for this model.

With a near-saturated model, the estimate of error will be fairly imprecise. Even with only a few terms being individually significant at the $\alpha = 0.05$ level, the overall sense is that this model is better than the two previous scenarios (based on R^2 and the mean square for error). Because the treatment effects aspect of the model is of more interest, we sequentially remove terms from the covariate portion of the model to add degrees of

Table 14-15 Minitab Analysis of Covariance for the Experiment in Table 14-14, Assuming a Common Slope

General Linear Model

Factor	Type	Levels	Values
A	fixed	2	-1 1
B	fixed	2	-1 1
C	fixed	2	-1 1

Analysis of Variance for y, using Adjusted SS for Tests

Source	DF	Seq SS	Adj SS	Adj MS	F	P
x	1	12155.9	2521.6	2521.6	28.10	0.001
A	1	1320.7	1403.8	1403.8	15.64	0.005
B	1	3997.6	4066.2	4066.2	45.31	0.000
C	1	52.7	82.3	82.3	0.92	0.370
A*B	1	3788.3	3641.0	3641.0	40.58	0.000
A*C	1	10.2	1.1	1.1	0.01	0.913
B*C	1	5.2	8.4	8.4	0.09	0.769
A*B*C	1	33.2	33.2	33.2	0.37	0.562
Error	7	628.1	628.1	89.7		
Total	15	21992.0				

Term	Coef	StDev	T	P
Constant	-1.016	5.454	-0.19	0.858
x	4.9245	0.9290	5.30	0.001

freedom to the estimate of error. If we sequentially remove the ACx term followed by BCx, the MS_E decreases to 0.7336 and several terms are insignificant. The final model is shown in Table 14-18 (on page 623) after sequentially removing Cx, AC, and BC.

This example emphasizes the need to have degrees of freedom available to estimate experimental error to increase the precision of the hypothesis tests associated with the individual terms in the model. This process should be done sequentially to avoid eliminating significant terms masked by a poor estimate of error.

Table 14-16 Minitab Analysis of Covariance, Reduced Model for the Experiment in Table 14-14

General Linear Model

Factor	Type	Levels	Values
A	fixed	2	-1 1
B	fixed	2	-1 1

Analysis of Variance for y, using Adjusted SS for Tests

Source	DF	Seq SS	Adj SS	Adj MS	F	P
x	1	12155.9	8287.9	8287.9	119.43	0.000
A	1	1320.7	1404.7	1404.7	20.24	0.001
B	1	3997.6	4097.7	4097.7	59.05	0.000
A*B	1	3754.5	3754.5	3754.5	54.10	0.000
Error	11	763.3	763.3	69.4		
Total	15	21992.0				

Term	Coef	StDev	T	P
Constant	-1.878	3.225	-0.58	0.572
x	5.0876	0.4655	10.93	0.000

Table 14-17 SAS PROC GLM Output (Analysis of Covariance) for the Experiment in Table 14-14

Dependent Variable: Y

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	13	21989.20828	1691.47756	1206.45	0.0008
Error	2	2.80406	1.40203		
Corrected Total	15	21992.01234			

R-Square	C.V.	Root MSE	Y Mean
0.999872	4.730820	1.184074	25.02895

Source	DF	Type III SS	Mean Square	F Value	Pr > F
A	1	4.6599694	4.6599694	3.32	0.2099
B	1	13.0525319	13.0525319	9.31	0.0927
C	1	35.0087994	35.0087994	24.97	0.0378
AB	1	17.1013635	17.1013635	12.20	0.0731
AC	1	0.0277472	0.0277472	0.02	0.9010
BC	1	0.4437474	0.4437474	0.32	0.6304
X	1	49.2741287	49.2741287	35.14	0.0273
AX	1	33.9024288	33.9024288	24.18	0.0390
BX	1	95.7747490	95.7747490	68.31	0.0143
CX	1	0.1283784	0.1283784	0.09	0.7908
ABX	1	336.9732676	336.9732676	240.35	0.0041
ACX	1	0.0020997	0.0020997	0.00	0.9726
BCX	1	0.0672386	0.0672386	0.05	0.8470

Table 14-18 SAS PROC GLM Output for the Experiment in Table 14-14, Reduced Model

Dependent Variable: Y

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	8	21986.33674	2748.29209	3389.61	0.0001
Error	7	5.67560	0.81080		
Corrected Total	15	21992.01234			

R-Square	C.V.	Root MSE	Y Mean
0.999742	3.597611	0.900444	25.02895

Source	DF	Type III SS	Mean Square	F Value	Pr > F
A	1	19.1597158	19.1597158	23.63	0.0018
B	1	38.0317496	38.0317496	46.91	0.0002
C	1	232.2435668	232.2435668	286.44	0.0001
AB	1	31.7635098	31.7635098	39.18	0.0004
X	1	240.8726525	240.8726525	297.08	0.0001
AX	1	233.3934567	233.3934567	287.86	0.0001
BX	1	550.1530561	550.1530561	678.53	0.0001
ABX	1	542.3268940	542.3268940	668.88	0.0001

Parameter	Estimate	T for H0: Parameter=0	Pr > |T|	Std Error of Estimate
Intercept	10.2438830	18.74	0.0001	0.54659908
A	2.7850330	4.86	0.0018	0.57291820
B	3.6596279	6.85	0.0002	0.53434356
C	5.4560862	16.92	0.0001	0.32237858
AB	-3.3636850	-6.26	0.0004	0.53741264
X	2.0471937	17.24	0.0001	0.11877417
AX	2.0632049	16.97	0.0001	0.12160595
BX	3.0340997	26.05	0.0001	0.11647826
ABX	-3.0342229	-25.86	0.0001	0.11732045

Reviewing the results obtained from the three approaches, we note that each method successively improves the model fit in this example. If there is a strong reason to believe that the covariate does not interact with the factors, it may be best to make that assumption at the outset of the analysis. This choice may also be dictated by software. Although experimental design software packages may only be able to model covariates that do not interact with treatments, the analyst may have a reasonable chance of identifying the major factors influencing the process, even if there is some covariate by treatment interaction. We also note that all the usual tests of model adequacy are still appropriate and are strongly recommended as part of the ANCOVA model building process.

14-4 REPEATED MEASURES

In experimental work in the social and behavioral sciences and some aspects of engineering and the physical sciences, the experimental units are frequently people. Because of differences in experience, training, or background, the differences in the responses of different people to the same treatment may be very large in some experimental situations. Unless it is controlled, this variability between people would become part of the experimental error, and in some cases, it would significantly inflate the error mean square, making it more difficult to detect real differences between treatments.

It is possible to control this variability between people by using a design in which each of the a treatments is used on each person (or "subject"). Such a design is called a **repeated measures design**. In this section we give a brief introduction to repeated measures experiments with a single factor.

Suppose that an experiment involves a treatments and every treatment is to be used exactly once on each of n subjects. The data would appear as in Table 14-19. Note that the observation y_{ij} represents the response of subject j to treatment i and that only n subjects are used. The model that we use for this design is

$$y_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij} \tag{14-45}$$

where τ_i is the effect of the ith treatment and β_j is a parameter associated with the jth subject. We assume that treatments are fixed (so $\sum_{i=1}^{a} \tau_i = 0$) and that the subjects employed are a random sample of subjects from some larger population of potential subjects. Thus, the subjects collectively represent a random effect, so we assume that the mean of β_j is zero and that the variance of β_j is σ_β^2. Because the term β_j is common to all a measurements on the same subject, the covariance between y_{ij} and $y_{i'j}$ is not, in general,

Table 14-19 Data for a Single-Factor Repeated Measures Design

	Subject				Treatment
Treatment	1	2	⋯	n	Totals
1	y_{11}	y_{12}	⋯	y_{1n}	$y_{1.}$
2	y_{21}	y_{22}	⋯	y_{2n}	$y_{2.}$
⋮	⋮	⋮		⋮	⋮
a	y_{a1}	y_{a2}		y_{an}	$y_{a.}$
Subject Totals	$y_{.1}$	$y_{.2}$	⋯	$y_{.n}$	$y_{..}$

zero. It is customary to assume that the covariance between y_{ij} and $y_{i'j}$ is constant across all treatments and subjects.

Consider an analysis of variance partitioning of the total sum of squares, say

$$\sum_{i=1}^{a}\sum_{j=1}^{n}(y_{ij}-\bar{y}_{..})^2 = a\sum_{j=1}^{n}(\bar{y}_{.j}-\bar{y}_{..})^2 + \sum_{i=1}^{a}\sum_{j=1}^{n}(y_{ij}-\bar{y}_{.j})^2 \qquad (14\text{-}46)$$

We may view the first term on the right-hand side of Equation 14-46 as a sum of squares that results from differences *between subjects* and the second term as a sum of squares of differences *within subjects*. That is,

$$SS_T = SS_{\text{Between Subjects}} + SS_{\text{Within Subjects}}$$

The sums of squares $SS_{\text{Between Subjects}}$ and $SS_{\text{Within Subjects}}$ are statistically independent, with degrees of freedom

$$an - 1 = (n - 1) + n(a - 1)$$

The differences within subjects depend on both differences in treatment effects and uncontrolled variability (noise or error). Therefore, we may decompose the sum of squares resulting from differences within subjects as follows:

$$\sum_{i=1}^{a}\sum_{j=1}^{n}(y_{ij}-\bar{y}_{.j})^2 = n\sum_{i=1}^{a}(\bar{y}_{i.}-\bar{y}_{..})^2 + \sum_{i=1}^{a}\sum_{j=1}^{n}(y_{ij}-\bar{y}_{i.}-\bar{y}_{.j}+\bar{y}_{..})^2 \qquad (14\text{-}47)$$

The first term on the right-hand side of Equation 14-47 measures the contribution of the difference between treatment means to $SS_{\text{Within Subjects}}$, and the second term is the residual variation due to error. Both components of $SS_{\text{Within Subjects}}$ are independent. Thus,

$$SS_{\text{Within Subjects}} = SS_{\text{Treatments}} + SS_E$$

with degrees of freedom given by

$$n(a - 1) = (a - 1) + (a - 1)(n - 1)$$

respectively.

To test the hypothesis of no treatment effect, that is,

$$H_0: \tau_1 = \tau_2 = \cdots = \tau_a = 0$$
$$H_1: \text{At least one } \tau_i \neq 0$$

we would use the ratio

$$F_0 = \frac{SS_{\text{Treatment}}/(a - 1)}{SS_E/(a - 1)(n - 1)} = \frac{MS_{\text{Treatments}}}{MS_E} \qquad (14\text{-}48)$$

If the model errors are normally distributed, then under the null hypothesis, $H_0: \tau_i = 0$, the statistic F_0 follows an $F_{a-1,(a-1)(n-1)}$ distribution. The null hypothesis would be rejected if $F_0 > F_{\alpha,a-1,(a-1)(n-1)}$.

The analysis of variance procedure is summarized in Table 14-20 (page 626), which also gives convenient computing formulas for the sums of squares. Readers should recognize the analysis of variance for a single-factor design with repeated measures as equivalent to the analysis for a randomized complete block design, with subjects considered to be the blocks.

Table 14-20 Analysis of Variance for a Single-Factor Repeated Measures Design

Source of Variation	Sums of Squares	Degrees of Freedom	Mean Square	F_0
1. Between subjects	$\sum_{j=1}^{n} \frac{y_{\cdot j}^2}{a} - \frac{y_{\cdot\cdot}^2}{an}$	$n - 1$		
2. Within subjects	$\sum_{i=1}^{a} \sum_{j=1}^{n} y_{ij}^2 - \sum_{j=1}^{n} \frac{y_{\cdot j}^2}{a}$	$n(a - 1)$		
3. (Treatments)	$\sum_{i=1}^{a} \frac{y_{i\cdot}^2}{n} - \frac{y_{\cdot\cdot}^2}{an}$	$a - 1$	$MS_{\text{Treatment}} = \frac{SS_{\text{Treatment}}}{a - 1}$	$\frac{MS_{\text{Treatment}}}{MS_E}$
4. (Error)	Subtraction: line (2) − line (3)	$(a - 1)(n - 1)$	$MS_E = \frac{SS_E}{(a - 1)(n - 1)}$	
5. Total	$\sum_{i=1}^{a} \sum_{j=1}^{n} y_{ij}^2 - \frac{y_{\cdot\cdot}^2}{an}$	$an - 1$		

14-5 PROBLEMS

14-1. Reconsider the experiment in Problem 5-22. Use the Box–Cox procedure to determine if a transformation on the response is appropriate (or useful) in the analysis of the data from this experiment.

14-2. In Example 6-3 we selected a log transformation for the drill advance rate response. Use the Box–Cox procedure to demonstrate that this is an appropriate data transformation.

14-3. Reconsider the smelting process experiment in Problem 8-23, where a 2^{6-3} fractional factorial design was used to study the weight of packing material that is stuck to carbon anodes after baking. Each of the eight runs in the design was replicated three times, and both the average weight and the range of the weights at each test combination were treated as response variables. Is there any indication that a transformation is required for either response?

14-4. In Problem 8-24 a replicated fractional factorial design was used to study substrate camber in semiconductor manufacturing. Both the mean and standard deviation of the camber measurements were used as response variables. Is there any indication that a transformation is required for either response?

14-5. Reconsider the photoresist experiment in Problem 8-25. Use the variance of the resist thickness at each test combination as the response variable. Is there any indication that a transformation is required?

14-6. In the grill defects experiment described in Problem 8-29, a variation of the square root transformation was employed in the analysis of the data. Use the Box–Cox method to determine if this is the appropriate transformation.

14-7. In the central composite design of Problem 11-14, two responses were obtained, the mean and variance of an oxide thickness. Use the Box–Cox method to investigate the potential usefulness of transformation for both of these responses. Is the log transformation suggested in part (c) of that problem appropriate?

14-8. In the 3^3 factorial design of Problem 11-33 one of the responses is a standard deviation. Use the Box–Cox method to investigate the usefulness of transformations for this response. Would your answer change if we used the variance as the response?

14-9. Problem 11-34 suggests using $\ln(s^2)$ as the response [refer to part (b)]. Does the Box–Cox method indicate that a transformation is appropriate?

14-10. A soft drink distributor is studying the effectiveness of delivery methods. Three different types of hand trucks have been developed, and an experiment is performed in the company's methods engineering laboratory. The variable of interest is the delivery time in minutes (y); however, delivery time is also strongly related to the case volume delivered (x). Each hand truck is used four times and the data that follow are obtained. Analyze these data and draw appropriate conclusions. Use $\alpha = 0.05$.

Hand Truck Type					
1		2		3	
y	x	y	x	y	x
27	24	25	26	40	38
44	40	35	32	22	26
33	35	46	42	53	50
41	40	26	25	18	20

14-11. Compute the adjusted treatment means and the standard errors of the adjusted treatment means for the data in Problem 14-10.

14-12. The sums of squares and products for a single-factor analysis of covariance follow. Complete the analysis and draw appropriate conclusions. Use $\alpha = 0.05$.

Source of Variation	Degrees of Freedom	Sums of Squares and Products		
		x	xy	y
Treatment	3	1500	1000	650
Error	12	6000	1200	550
Total	15	7500	2200	1200

14-13. Find the standard errors of the adjusted treatment means in Example 14-4.

14-14. Four different formulations of an industrial glue are being tested. The tensile strength of the glue when it is applied to join parts is also related to the application thickness. Five observations on strength (y) in pounds and thickness (x) in 0.01 inches are obtained for each formulation. The data are shown in the following table. Analyze these data and draw appropriate conclusions.

Glue Formulation							
1		2		3		4	
y	x	y	x	y	x	y	x
46.5	13	48.7	12	46.3	15	44.7	16
45.9	14	49.0	10	47.1	14	43.0	15
49.8	12	50.1	11	48.9	11	51.0	10
46.1	12	48.5	12	48.2	11	48.1	12
44.3	14	45.2	14	50.3	10	48.6	11

14-15. Compute the adjusted treatment means and their standard errors using the data in Problem 14-14.

14-16. An engineer is studying the effect of cutting speed on the rate of metal removal in a machining operation. However, the rate of metal removal is also related to the hardness of the test specimen. Five observations are taken at each cutting speed. The amount of metal removed (y) and the hardness of the specimen (x) are shown in the following table. Analyze the data using an analysis of covariance. Use $\alpha = 0.05$.

Cutting Speed (rpm)					
1000		1200		1400	
y	x	y	x	y	x
68	120	112	165	118	175
90	140	94	140	82	132
98	150	65	120	73	124
77	125	74	125	92	141
88	136	85	133	80	130

14-17. Show that in a single-factor analysis of covariance with a single covariate a $100(1 - \alpha)$ percent confidence interval on the ith adjusted treatment mean is

$$\bar{y}_{i.} - \hat{\beta}(\bar{x}_{i.} - \bar{x}_{..}) \pm t_{\alpha/2,a(n-1)-1}\left[MS_E\left(\frac{1}{n} + \frac{(\bar{x}_{i.} - \bar{x}_{..})^2}{E_{xx}}\right)\right]^{1/2}$$

Using this formula, calculate a 95 percent confidence interval on the adjusted mean of machine 1 in Example 14-4.

14-18. Show that in a single-factor analysis of covariance with a single covariate, the standard error of the difference between any two adjusted treatment means is

$$S_{\text{Adj}\bar{y}_{i.}-\text{Adj}\bar{y}_{j.}} = \left[MS_E \left(\frac{2}{n} + \frac{(\bar{x}_{i.} - \bar{x}_{j.})^2}{E_{xx}} \right) \right]^{1/2}$$

14-19. Discuss how the operating characteristic curves for the analysis of variance can be used in the analysis of covariance.

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Appendix

I. Cumulative Standard Normal Distribution

II. Percentage Points of the t Distribution

III. Percentage Points of the χ^2 Distribution

IV. Percentage Points of the F Distribution

V. Operating Characteristic Curves for the Fixed Effects Model Analysis of Variance

VI. Operating Characteristic Curves for the Random Effects Model Analysis of Variance

VII. Significant Ranges for Duncan's Multiple Range Test

VIII. Percentage Points of the Studentized Range Statistic

IX. Critical Values for Dunnett's Test for Comparing Treatments with a Control

X. Coefficients of Orthogonal Polynomials

XI. Random Numbers

XII. Alias Relationships for 2^{k-p} Fractional Factorial Designs with $k \leq 15$ and $n \leq 64$

I. Cumulative Standard Normal Distribution[a]

$$\Phi(z) = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} e^{-u^2/2}\, du$$

z	.00	.01	.02	.03	.04	z
.0	.50000	.50399	.50798	.51197	.51595	0
.1	.53983	.54379	.54776	.55172	.55567	.1
.2	.57926	.58317	.58706	.59095	.59483	.2
.3	.61791	.62172	.62551	.62930	.63307	.3
.4	.65542	.65910	.66276	.66640	.67003	.4
.5	.69146	.69497	.69847	.70194	.70540	.5
.6	.72575	.72907	.73237	.73565	.73891	.6
.7	.75803	.76115	.76424	.76730	.77035	.7
.8	.78814	.79103	.79389	.79673	.79954	.8
.9	.81594	.81859	.82121	.82381	.82639	.9
1.0	.84134	.84375	.84613	.84849	.85083	1.0
1.1	.86433	.86650	.86864	.87076	.87285	1.1
1.2	.88493	.88686	.88877	.89065	.89251	1.2
1.3	.90320	.90490	.90658	.90824	.90988	1.3
1.4	.91924	.92073	.92219	.92364	.92506	1.4
1.5	.93319	.93448	.93574	.93699	.93822	1.5
1.6	.94520	.94630	.94738	.94845	.94950	1.6
1.7	.95543	.95637	.95728	.95818	.95907	1.7
1.8	.96407	.96485	.96562	.96637	.96711	1.8
1.9	.97128	.97193	.97257	.97320	.97381	1.9
2.0	.97725	.97778	.97831	.97882	.97932	2.0
2.1	.98214	.98257	.98300	.98341	.93882	2.1
2.2	.98610	.98645	.98679	.98713	.98745	2.2
2.3	.98928	.98956	.98983	.99010	.99036	2.3
2.4	.99180	.99202	.99224	.99245	.99266	2.4
2.5	.99379	.99396	.99413	.99430	.99446	2.5
2.6	.99534	.99547	.99560	.99573	.99585	2.6
2.7	.99653	.99664	.99674	.99683	.99693	2.7
2.8	.99744	.99752	.99760	.99767	.99774	2.8
2.9	.99813	.99819	.99825	.99831	.99836	2.9
3.0	.99865	.99869	.99874	.99878	.99882	3.0
3.1	.99903	.99906	.99910	.99913	.99916	3.1
3.2	.99931	.99934	.99936	.99938	.99940	3.2
3.3	.99952	.99953	.99955	.99957	.99958	3.3
3.4	.99966	.99968	.99969	.99970	.99971	3.4
3.5	.99977	.99978	.99978	.99979	.99980	3.5
3.6	.99984	.99985	.99985	.99986	.99986	3.6
3.7	.99989	.99990	.99990	.99990	.99991	3.7
3.8	.99993	.99993	.99993	.99994	.99994	3.8
3.9	.99995	.99995	.99996	.99996	.99996	3.9

[a] Reproduced with permission from *Probability and Statistics in Engineering and Management Science*, 3rd edition, by W. W. Hines and D. C. Montgomery, Wiley, New York, 1990.

I. Cumulative Standard Normal Distribution (*continued*)

$$\Phi(z) = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} e^{-u^2/2}\, du$$

z	.05	.06	.07	.08	.09	z
.0	.51994	.52392	.52790	.53188	.53586	.0
.1	.55962	.56356	.56749	.57142	.57534	.1
.2	.59871	.60257	.60642	.61026	.61409	.2
.3	.63683	.64058	.64431	.64803	.65173	.3
.4	.67364	.67724	.68082	.68438	.68793	.4
.5	.70884	.71226	.71566	.71904	.72240	.5
.6	.74215	.74537	.74857	.75175	.75490	.6
.7	.77337	.77637	.77935	.78230	.78523	.7
.8	.80234	.80510	.80785	.81057	.81327	.8
.9	.82894	.83147	.83397	.83646	.83891	.9
1.0	.85314	.85543	.85769	.85993	.86214	1.0
1.1	.87493	.87697	.87900	.88100	.88297	1.1
1.2	.89435	.89616	.89796	.89973	.90147	1.2
1.3	.91149	.91308	.91465	.91621	.91773	1.3
1.4	.92647	.92785	.92922	.93056	.93189	1.4
1.5	.93943	.90462	.94179	.94295	.94408	1.5
1.6	.95053	.95154	.95254	.95352	.95448	1.6
1.7	.95994	.96080	.96164	.96246	.96327	1.7
1.8	.96784	.96856	.96926	.96995	.97062	1.8
1.9	.97441	.97500	.97558	.97615	.97670	1.9
2.0	.97982	.98030	.98077	.98124	.98169	2.0
2.1	.98422	.98461	.98500	.98537	.98574	2.1
2.2	.98778	.98809	.98840	.98870	.98899	2.2
2.3	.99061	.99086	.99111	.99134	.99158	2.3
2.4	.99286	.99305	.99324	.99343	.99361	2.4
2.5	.99461	.99477	.99492	.99506	.99520	2.5
2.6	.99598	.99609	.99621	.99632	.99643	2.6
2.7	.99702	.99711	.99720	.99728	.99736	2.7
2.8	.99781	.99788	.99795	.99801	.99807	2.8
2.9	.99841	.99846	.99851	.99856	.99861	2.9
3.0	.99886	.99889	.99893	.99897	.99900	3.0
3.1	.99918	.99921	.99924	.99926	.99929	3.1
3.2	.99942	.99944	.99946	.99948	.99950	3.2
3.3	.99960	.99961	.99962	.99964	.99965	3.3
3.4	.99972	.99973	.99974	.99975	.99976	3.4
3.5	.99981	.99981	.99982	.99983	.99983	3.5
3.6	.99987	.99987	.99988	.99988	.99989	3.6
3.7	.99991	.99992	.99992	.99992	.99992	3.7
3.8	.99994	.99994	.99995	.99995	.99995	3.8
3.9	.99996	.99996	.99996	.99997	.99997	3.9

II. Percentage Points of the t Distribution[a]

ν \ α	.40	.25	.10	.05	.025	.01	.005	.0025	.001	.0005
1	.325	1.000	3.078	6.314	12.706	31.821	63.657	127.32	318.31	636.62
2	.289	.816	1.886	2.920	4.303	6.965	9.925	14.089	23.326	31.598
3	.277	.765	1.638	2.353	3.182	4.541	5.841	7.453	10.213	12.924
4	.271	.741	1.533	2.132	2.776	3.747	4.604	5.598	7.173	8.610
5	.267	.727	1.476	2.015	2.571	3.365	4.032	4.773	5.893	6.869
6	.265	.727	1.440	1.943	2.447	3.143	3.707	4.317	5.208	5.959
7	.263	.711	1.415	1.895	2.365	2.998	3.499	4.019	4.785	5.408
8	.262	.706	1.397	1.860	2.306	2.896	3.355	3.833	4.501	5.041
9	.261	.703	1.383	1.833	2.262	2.821	3.250	3.690	4.297	4.781
10	.260	.700	1.372	1.812	2.228	2.764	3.169	3.581	4.144	4.587
11	.260	.697	1.363	1.796	2.201	2.718	3.106	3.497	4.025	4.437
12	.259	.695	1.356	1.782	2.179	2.681	3.055	3.428	3.930	4.318
13	.259	.694	1.350	1.771	2.160	2.650	3.012	3.372	3.852	4.221
14	.258	.692	1.345	1.761	2.145	2.624	2.977	3.326	3.787	4.140
15	.258	.691	1.341	1.753	2.131	2.602	2.947	3.286	3.733	4.073
16	.258	.690	1.337	1.746	2.120	2.583	2.921	3.252	3.686	4.015
17	.257	.689	1.333	1.740	2.110	2.567	2.898	3.222	3.646	3.965
18	.257	.688	1.330	1.734	2.101	2.552	2.878	3.197	3.610	3.922
19	.257	.688	1.328	1.729	2.093	2.539	2.861	3.174	3.579	3.883
20	.257	.687	1.325	1.725	2.086	2.528	2.845	3.153	3.552	3.850
21	.257	.686	1.323	1.721	2.080	2.518	2.831	3.135	3.527	3.819
22	.256	.686	1.321	1.717	2.074	2.508	2.819	3.119	3.505	3.792
23	.256	.685	1.319	1.714	2.069	2.500	2.807	3.104	3.485	3.767
24	.256	.685	1.318	1.711	2.064	2.492	2.797	3.091	3.467	3.745
25	.256	.684	1.316	1.708	2.060	2.485	2.787	3.078	3.450	3.725
26	.256	.684	1.315	1.706	2.056	2.479	2.779	3.067	3.435	3.707
27	.256	.684	1.314	1.703	2.052	2.473	2.771	3.057	3.421	3.690
28	.256	.683	1.313	1.701	2.048	2.467	2.763	3.047	3.408	3.674
29	.256	.683	1.311	1.699	2.045	2.462	2.756	3.038	3.396	3.659
30	.256	.683	1.310	1.697	2.042	2.457	2.750	3.030	3.385	3.646
40	.255	.681	1.303	1.684	2.021	2.423	2.704	2.971	3.307	3.551
60	.254	.679	1.296	1.671	2.000	2.390	2.660	2.915	3.232	3.460
120	.254	.677	1.289	1.658	1.980	2.358	2.617	2.860	3.160	3.373
∞	.253	.674	1.282	1.645	1.960	2.326	2.576	2.807	3.090	3.291

ν = degrees of freedom.

[a] Adapted with permission from *Biometrika Tables for Statisticians*, Vol. 1, 3rd edition, by E. S. Pearson and H. O. Hartley, Cambridge University Press, Cambridge, 1966.

III. Percentage Points of the χ^2 Distribution[a]

ν	α .995	.990	.975	.950	.500	.050	.025	.010	.005
1	0.00 +	0.00 +	0.00 +	0.00 +	0.45	3.84	5.02	6.63	7.88
2	0.01	0.02	0.05	0.10	1.39	5.99	7.38	9.21	10.60
3	0.07	0.11	0.22	0.35	2.37	7.81	9.35	11.34	12.84
4	0.21	0.30	0.48	0.71	3.36	9.49	11.14	13.28	14.86
5	0.41	0.55	0.83	1.15	4.35	11.07	12.38	15.09	16.75
6	0.68	0.87	1.24	1.64	5.35	12.59	14.45	16.81	18.55
7	0.99	1.24	1.69	2.17	6.35	14.07	16.01	18.48	20.28
8	1.34	1.65	2.18	2.73	7.34	15.51	17.53	20.09	21.96
9	1.73	2.09	2.70	3.33	8.34	16.92	19.02	21.67	23.59
10	2.16	2.56	3.25	3.94	9.34	18.31	20.48	23.21	25.19
11	2.60	3.05	3.82	4.57	10.34	19.68	21.92	24.72	26.76
12	3.07	3.57	4.40	5.23	11.34	21.03	23.34	26.22	28.30
13	3.57	4.11	5.01	5.89	12.34	22.36	24.74	27.69	29.82
14	4.07	4.66	5.63	6.57	13.34	23.68	26.12	29.14	31.32
15	4.60	5.23	6.27	7.26	14.34	25.00	27.49	30.58	32.80
16	5.14	5.81	6.91	7.96	15.34	26.30	28.85	32.00	34.27
17	5.70	6.41	7.56	8.67	16.34	27.59	30.19	33.41	35.72
18	6.26	7.01	8.23	9.39	17.34	28.87	31.53	34.81	37.16
19	6.84	7.63	8.91	10.12	18.34	30.14	32.85	36.19	38.58
20	7.43	8.26	9.59	10.85	19.34	31.41	34.17	37.57	40.00
25	10.52	11.52	13.12	14.61	24.34	37.65	40.65	44.31	46.93
30	13.79	14.95	16.79	18.49	29.34	43.77	46.98	50.89	53.67
40	20.71	22.16	24.43	26.51	39.34	55.76	59.34	63.69	66.77
50	27.99	29.71	32.36	34.76	49.33	67.50	71.42	76.15	79.49
60	35.53	37.48	40.48	43.19	59.33	79.08	83.30	88.38	91.95
70	43.28	45.44	48.76	51.74	69.33	90.53	95.02	100.42	104.22
80	51.17	53.54	57.15	60.39	79.33	101.88	106.63	112.33	116.32
90	59.20	61.75	65.65	69.13	89.33	113.14	118.14	124.12	128.30
100	67.33	70.06	74.22	77.93	99.33	124.34	129.56	135.81	140.17

ν = degrees of freedom

[a] Adapted with permission from *Biometrika Tables for Statisticians*, Vol. 1, 3rd edition by E. S. Pearson and H. O. Hartley, Cambridge University Press, Cambridge, 1966.

ν_2 \ ν_1	1	2	3	4	5	6	7	8	9	10	12	15	20	24	30	40	60	120	∞
	Degrees of Freedom for the Numerator (ν_1)																		
Degrees of Freedom for the Denominator (ν_2)																			
1	5.83	7.50	8.20	8.58	8.82	8.98	9.10	9.19	9.26	9.32	9.41	9.49	9.58	9.63	9.67	9.71	9.76	9.80	9.85
2	2.57	3.00	3.15	3.23	3.28	3.31	3.34	3.35	3.37	3.38	3.39	3.41	3.43	3.43	3.44	3.45	3.46	3.47	3.48
3	2.02	2.28	2.36	2.39	2.41	2.42	2.43	2.44	2.44	2.44	2.45	2.46	2.46	2.46	2.47	2.47	2.47	2.47	2.47
4	1.81	2.00	2.05	2.06	2.07	2.08	2.08	2.08	2.08	2.08	2.08	2.08	2.08	2.08	2.08	2.08	2.08	2.08	2.08
5	1.69	1.85	1.88	1.89	1.89	1.89	1.89	1.89	1.89	1.89	1.89	1.89	1.88	1.88	1.88	1.88	1.87	1.87	1.87
6	1.62	1.76	1.78	1.79	1.79	1.78	1.78	1.78	1.77	1.77	1.77	1.76	1.76	1.75	1.75	1.75	1.74	1.74	1.74
7	1.57	1.70	1.72	1.72	1.71	1.71	1.70	1.70	1.70	1.69	1.68	1.68	1.67	1.67	1.66	1.66	1.65	1.65	1.65
8	1.54	1.66	1.67	1.66	1.66	1.65	1.64	1.64	1.63	1.63	1.62	1.62	1.61	1.60	1.60	1.59	1.59	1.58	1.58
9	1.51	1.62	1.63	1.63	1.62	1.61	1.60	1.60	1.59	1.59	1.58	1.57	1.56	1.56	1.55	1.54	1.54	1.53	1.53
10	1.49	1.60	1.60	1.59	1.59	1.58	1.57	1.56	1.56	1.55	1.54	1.53	1.52	1.52	1.51	1.51	1.50	1.49	1.48
11	1.47	1.58	1.58	1.57	1.56	1.55	1.54	1.53	1.53	1.52	1.51	1.50	1.49	1.49	1.48	1.47	1.47	1.46	1.45
12	1.46	1.56	1.56	1.55	1.54	1.53	1.52	1.51	1.51	1.50	1.49	1.48	1.47	1.46	1.45	1.45	1.44	1.43	1.42
13	1.45	1.55	1.55	1.53	1.52	1.51	1.50	1.49	1.49	1.48	1.47	1.46	1.45	1.44	1.43	1.42	1.42	1.41	1.40
14	1.44	1.53	1.53	1.52	1.51	1.50	1.49	1.48	1.47	1.46	1.45	1.44	1.43	1.42	1.41	1.41	1.40	1.39	1.38
15	1.43	1.52	1.52	1.51	1.49	1.48	1.47	1.46	1.46	1.45	1.44	1.43	1.41	1.41	1.40	1.39	1.38	1.37	1.36
16	1.42	1.51	1.51	1.50	1.48	1.47	1.46	1.45	1.44	1.44	1.43	1.41	1.40	1.39	1.38	1.37	1.36	1.35	1.34
17	1.42	1.51	1.50	1.49	1.47	1.46	1.45	1.44	1.43	1.43	1.41	1.40	1.39	1.38	1.37	1.36	1.35	1.34	1.33
18	1.41	1.50	1.49	1.48	1.46	1.45	1.44	1.43	1.42	1.42	1.40	1.39	1.38	1.37	1.36	1.35	1.34	1.33	1.32
19	1.41	1.49	1.49	1.47	1.46	1.44	1.43	1.42	1.41	1.41	1.40	1.38	1.37	1.36	1.35	1.34	1.33	1.32	1.30
20	1.40	1.49	1.48	1.47	1.45	1.44	1.43	1.42	1.41	1.40	1.39	1.37	1.36	1.35	1.34	1.33	1.32	1.31	1.29
21	1.40	1.48	1.48	1.46	1.44	1.43	1.42	1.41	1.40	1.39	1.38	1.37	1.35	1.34	1.33	1.32	1.31	1.30	1.28
22	1.40	1.48	1.47	1.45	1.44	1.42	1.41	1.40	1.39	1.39	1.37	1.36	1.34	1.33	1.32	1.31	1.30	1.29	1.28
23	1.39	1.47	1.47	1.45	1.43	1.42	1.41	1.40	1.39	1.38	1.37	1.35	1.34	1.33	1.32	1.31	1.30	1.28	1.27
24	1.39	1.47	1.46	1.44	1.43	1.41	1.40	1.39	1.38	1.38	1.36	1.35	1.33	1.32	1.31	1.30	1.29	1.28	1.26
25	1.39	1.47	1.46	1.44	1.42	1.41	1.40	1.39	1.38	1.37	1.36	1.34	1.33	1.32	1.31	1.29	1.28	1.27	1.25
26	1.38	1.46	1.45	1.44	1.42	1.41	1.39	1.38	1.37	1.37	1.35	1.34	1.32	1.31	1.30	1.29	1.28	1.26	1.25
27	1.38	1.46	1.45	1.43	1.42	1.40	1.39	1.38	1.37	1.36	1.35	1.33	1.32	1.31	1.30	1.28	1.27	1.26	1.24
28	1.38	1.46	1.45	1.43	1.41	1.40	1.39	1.38	1.37	1.36	1.34	1.33	1.31	1.30	1.29	1.28	1.27	1.25	1.24
29	1.38	1.45	1.45	1.43	1.41	1.40	1.38	1.37	1.36	1.35	1.34	1.32	1.31	1.30	1.29	1.27	1.26	1.25	1.23
30	1.38	1.45	1.44	1.42	1.41	1.39	1.38	1.37	1.36	1.35	1.34	1.32	1.30	1.29	1.28	1.27	1.26	1.24	1.23
40	1.36	1.44	1.42	1.40	1.39	1.37	1.36	1.35	1.34	1.33	1.31	1.30	1.28	1.26	1.25	1.24	1.22	1.21	1.19
60	1.35	1.42	1.41	1.38	1.37	1.35	1.33	1.32	1.31	1.30	1.29	1.27	1.25	1.24	1.22	1.21	1.19	1.17	1.15
120	1.34	1.40	1.39	1.37	1.35	1.33	1.31	1.30	1.29	1.28	1.26	1.24	1.22	1.21	1.19	1.18	1.16	1.13	1.10
∞	1.32	1.39	1.37	1.35	1.33	1.31	1.29	1.28	1.27	1.25	1.24	1.22	1.19	1.18	1.16	1.14	1.12	1.08	1.00

ν_2 \ ν_1	1	2	3	4	5	6	7	8	9	10	12	15	20	24	30	40	60	120	∞
1	39.86	49.50	53.59	55.83	57.24	58.20	58.91	59.44	59.86	60.19	60.71	61.22	61.74	62.00	62.26	62.53	62.79	63.06	63.33
2	8.53	9.00	9.16	9.24	9.29	9.33	9.35	9.37	9.38	9.39	9.41	9.42	9.44	9.45	9.46	9.47	9.47	9.48	9.49
3	5.54	5.46	5.39	5.34	5.31	5.28	5.27	5.25	5.24	5.23	5.22	5.20	5.18	5.18	5.17	5.16	5.15	5.14	5.13
4	4.54	4.32	4.19	4.11	4.05	4.01	3.98	3.95	3.94	3.92	3.90	3.87	3.84	3.83	3.82	3.80	3.79	3.78	3.76
5	4.06	3.78	3.62	3.52	3.45	3.40	3.37	3.34	3.32	3.30	3.27	3.24	3.21	3.19	3.17	3.16	3.14	3.12	3.10
6	3.78	3.46	3.29	3.18	3.11	3.05	3.01	2.98	2.96	2.94	2.90	2.87	2.84	2.82	2.80	2.78	2.76	2.74	2.72
7	3.59	3.26	3.07	2.96	2.88	2.83	2.78	2.75	2.72	2.70	2.67	2.63	2.59	2.58	2.56	2.54	2.51	2.49	2.47
8	3.46	3.11	2.92	2.81	2.73	2.67	2.62	2.59	2.56	2.54	2.50	2.46	2.42	2.40	2.38	2.36	2.34	2.32	2.29
9	3.36	3.01	2.81	2.69	2.61	2.55	2.51	2.47	2.44	2.42	2.38	2.34	2.30	2.28	2.25	2.23	2.21	2.18	2.16
10	3.29	2.92	2.73	2.61	2.52	2.46	2.41	2.38	2.35	2.32	2.28	2.24	2.20	2.18	2.16	2.13	2.11	2.08	2.06
11	3.23	2.86	2.66	2.54	2.45	2.39	2.34	2.30	2.27	2.25	2.21	2.17	2.12	2.10	2.08	2.05	2.03	2.00	1.97
12	3.18	2.81	2.61	2.48	2.39	2.33	2.28	2.24	2.21	2.19	2.15	2.10	2.06	2.04	2.01	1.99	1.96	1.93	1.90
13	3.14	2.76	2.56	2.43	2.35	2.28	2.23	2.20	2.16	2.14	2.10	2.05	2.01	1.98	1.96	1.93	1.90	1.88	1.85
14	3.10	2.73	2.52	2.39	2.31	2.24	2.19	2.15	2.12	2.10	2.05	2.01	1.96	1.94	1.91	1.89	1.86	1.83	1.80
15	3.07	2.70	2.49	2.36	2.27	2.21	2.16	2.12	2.09	2.06	2.02	1.97	1.92	1.90	1.87	1.85	1.82	1.79	1.76
16	3.05	2.67	2.46	2.33	2.24	2.18	2.13	2.09	2.06	2.03	1.99	1.94	1.89	1.87	1.84	1.81	1.78	1.75	1.72
17	3.03	2.64	2.44	2.31	2.22	2.15	2.10	2.06	2.03	2.00	1.96	1.91	1.86	1.84	1.81	1.78	1.75	1.72	1.69
18	3.01	2.62	2.42	2.29	2.20	2.13	2.08	2.04	2.00	1.98	1.93	1.89	1.84	1.81	1.78	1.75	1.72	1.69	1.66
19	2.99	2.61	2.40	2.27	2.18	2.11	2.06	2.02	1.98	1.96	1.91	1.86	1.81	1.79	1.76	1.73	1.70	1.67	1.63
20	2.97	2.59	2.38	2.25	2.16	2.09	2.04	2.00	1.96	1.94	1.89	1.84	1.79	1.77	1.74	1.71	1.68	1.64	1.61
21	2.96	2.57	2.36	2.23	2.14	2.08	2.02	1.98	1.95	1.92	1.87	1.83	1.78	1.75	1.72	1.69	1.66	1.62	1.59
22	2.95	2.56	2.35	2.22	2.13	2.06	2.01	1.97	1.93	1.90	1.86	1.81	1.76	1.73	1.70	1.67	1.64	1.60	1.57
23	2.94	2.55	2.34	2.21	2.11	2.05	1.99	1.96	1.92	1.89	1.84	1.80	1.74	1.72	1.69	1.66	1.62	1.59	1.55
24	2.93	2.54	2.33	2.19	2.10	2.04	1.98	1.94	1.91	1.88	1.83	1.78	1.73	1.70	1.67	1.64	1.61	1.57	1.53
25	2.92	2.53	2.32	2.18	2.09	2.02	1.97	1.93	1.89	1.87	1.82	1.77	1.72	1.69	1.66	1.63	1.59	1.56	1.52
26	2.91	2.52	2.31	2.17	2.08	2.01	1.96	1.92	1.88	1.86	1.81	1.76	1.71	1.68	1.65	1.61	1.58	1.54	1.50
27	2.90	2.51	2.30	2.17	2.07	2.00	1.95	1.91	1.87	1.85	1.80	1.75	1.70	1.67	1.64	1.60	1.57	1.53	1.49
28	2.89	2.50	2.29	2.16	2.06	2.00	1.94	1.90	1.87	1.84	1.79	1.74	1.69	1.66	1.63	1.59	1.56	1.52	1.48
29	2.89	2.50	2.28	2.15	2.06	1.99	1.93	1.89	1.86	1.83	1.78	1.73	1.68	1.65	1.62	1.58	1.55	1.51	1.47
30	2.88	2.49	2.28	2.14	2.03	1.98	1.93	1.88	1.85	1.82	1.77	1.72	1.67	1.64	1.61	1.57	1.54	1.50	1.46
40	2.84	2.44	2.23	2.09	2.00	1.93	1.87	1.83	1.79	1.76	1.71	1.66	1.61	1.57	1.54	1.51	1.47	1.42	1.38
60	2.79	2.39	2.18	2.04	1.95	1.87	1.82	1.77	1.74	1.71	1.66	1.60	1.54	1.51	1.48	1.44	1.40	1.35	1.29
120	2.75	2.35	2.13	1.99	1.90	1.82	1.77	1.72	1.68	1.65	1.60	1.55	1.48	1.45	1.41	1.37	1.32	1.26	1.19
∞	2.71	2.30	2.08	1.94	1.85	1.77	1.72	1.67	1.63	1.60	1.55	1.49	1.42	1.38	1.34	1.30	1.24	1.17	1.00

Degrees of Freedom for the Numerator (ν_1)

Degrees of Freedom for the Denominator (ν_2)

ν_2 \ ν_1	1	2	3	4	5	6	7	8	9	10	12	15	20	24	30	40	60	120	∞
	161.4	199.5	215.7	224.6	230.2	234.0	236.8	238.9	240.5	241.9	243.9	245.9	248.0	249.1	250.1	251.1	252.2	253.3	254.3
2	18.51	19.00	19.16	19.25	19.30	19.33	19.35	19.37	19.38	19.40	19.41	19.43	19.45	19.45	19.46	19.47	19.48	19.49	19.50
3	10.13	9.55	9.28	9.12	9.01	8.94	8.89	8.85	8.81	8.79	8.74	8.70	8.66	8.64	8.62	8.59	8.57	8.55	8.53
4	7.71	6.94	6.59	6.39	6.26	6.16	6.09	6.04	6.00	5.96	5.91	5.86	5.80	5.77	5.75	5.72	5.69	5.66	5.63
5	6.61	5.79	5.41	5.19	5.05	4.95	4.88	4.82	4.77	4.74	4.68	4.62	4.56	4.53	4.50	4.46	4.43	4.40	4.36
6	5.99	5.14	4.76	4.53	4.39	4.28	4.21	4.15	4.10	4.06	4.00	3.94	3.87	3.84	3.81	3.77	3.74	3.70	3.67
7	5.59	4.74	4.35	4.12	3.97	3.87	3.79	3.73	3.68	3.64	3.57	3.51	3.44	3.41	3.38	3.34	3.30	3.27	3.23
8	5.32	4.46	4.07	3.84	3.69	3.58	3.50	3.44	3.39	3.35	3.28	3.22	3.15	3.12	3.08	3.04	3.01	2.97	2.93
9	5.12	4.26	3.86	3.63	3.48	3.37	3.29	3.23	3.18	3.14	3.07	3.01	2.94	2.90	2.86	2.83	2.79	2.75	2.71
10	4.96	4.10	3.71	3.48	3.33	3.22	3.14	3.07	3.02	2.98	2.91	2.85	2.77	2.74	2.70	2.66	2.62	2.58	2.54
11	4.84	3.98	3.59	3.36	3.20	3.09	3.01	2.95	2.90	2.85	2.79	2.72	2.65	2.61	2.57	2.53	2.49	2.45	2.40
12	4.75	3.89	3.49	3.26	3.11	3.00	2.91	2.85	2.80	2.75	2.69	2.62	2.54	2.51	2.47	2.43	2.38	2.34	2.30
13	4.67	3.81	3.41	3.18	3.03	2.92	2.83	2.77	2.71	2.67	2.60	2.53	2.46	2.42	2.38	2.34	2.30	2.25	2.21
14	4.60	3.74	3.34	3.11	2.96	2.85	2.76	2.70	2.65	2.60	2.53	2.46	2.39	2.35	2.31	2.27	2.22	2.18	2.13
15	4.54	3.68	3.29	3.06	2.90	2.79	2.71	2.64	2.59	2.54	2.48	2.40	2.33	2.29	2.25	2.20	2.16	2.11	2.07
16	4.49	3.63	3.24	3.01	2.85	2.74	2.66	2.59	2.54	2.49	2.42	2.35	2.28	2.24	2.19	2.15	2.11	2.06	2.01
17	4.45	3.59	3.20	2.96	2.81	2.70	2.61	2.55	2.49	2.45	2.38	2.31	2.23	2.19	2.15	2.10	2.06	2.01	1.96
18	4.41	3.55	3.16	2.93	2.77	2.66	2.58	2.51	2.46	2.41	2.34	2.27	2.19	2.15	2.11	2.06	2.02	1.97	1.92
19	4.38	3.52	3.13	2.90	2.74	2.63	2.54	2.48	2.42	2.38	2.31	2.23	2.16	2.11	2.07	2.03	1.98	1.93	1.88
20	4.35	3.49	3.10	2.87	2.71	2.60	2.51	2.45	2.39	2.35	2.28	2.20	2.12	2.08	2.04	1.99	1.95	1.90	1.84
21	4.32	3.47	3.07	2.84	2.68	2.57	2.49	2.42	2.37	2.32	2.25	2.18	2.10	2.05	2.01	1.96	1.92	1.87	1.81
22	4.30	3.44	3.05	2.82	2.66	2.55	2.46	2.40	2.34	2.30	2.23	2.15	2.07	2.03	1.98	1.94	1.89	1.84	1.78
23	4.28	3.42	3.03	2.80	2.64	2.53	2.44	2.37	2.32	2.27	2.20	2.13	2.05	2.01	1.96	1.91	1.86	1.81	1.76
24	4.26	3.40	3.01	2.78	2.62	2.51	2.42	2.36	2.30	2.25	2.18	2.11	2.03	1.98	1.94	1.89	1.84	1.79	1.73
25	4.24	3.39	2.99	2.76	2.60	2.49	2.40	2.34	2.28	2.24	2.16	2.09	2.01	1.96	1.92	1.87	1.82	1.77	1.71
26	4.23	3.37	2.98	2.74	2.59	2.47	2.39	2.32	2.27	2.22	2.15	2.07	1.99	1.95	1.90	1.85	1.80	1.75	1.69
27	4.21	3.35	2.96	2.73	2.57	2.46	2.37	2.31	2.25	2.20	2.13	2.06	1.97	1.93	1.88	1.84	1.79	1.73	1.67
28	4.20	3.34	2.95	2.71	2.56	2.45	2.36	2.29	2.24	2.19	2.12	2.04	1.96	1.91	1.87	1.82	1.77	1.71	1.65
29	4.18	3.33	2.93	2.70	2.55	2.43	2.35	2.28	2.22	2.18	2.10	2.03	1.94	1.90	1.85	1.81	1.75	1.70	1.64
30	4.17	3.32	2.92	2.69	2.53	2.42	2.33	2.27	2.21	2.16	2.09	2.01	1.93	1.89	1.84	1.79	1.74	1.68	1.62
40	4.08	3.23	2.84	2.61	2.45	2.34	2.25	2.18	2.12	2.08	2.00	1.92	1.84	1.79	1.74	1.69	1.64	1.58	1.51
60	4.00	3.15	2.76	2.53	2.37	2.25	2.17	2.10	2.04	1.99	1.92	1.84	1.75	1.70	1.65	1.59	1.53	1.47	1.39
120	3.92	3.07	2.68	2.45	2.29	2.17	2.09	2.02	1.96	1.91	1.83	1.75	1.66	1.61	1.55	1.55	1.43	1.35	1.25

Degrees of Freedom for the Numerator (ν_1)

Degrees of Freedom for the Denominator (ν_2)

ν_2 \ ν_1	Degrees of Freedom for the Numerator (ν_1)																		
	1	2	3	4	5	6	7	8	9	10	12	15	20	24	30	40	60	120	∞
1	647.8	799.5	864.2	899.6	921.8	937.1	948.2	956.7	963.3	968.6	976.7	984.9	993.1	997.2	1001	1006	1010	1014	1018
2	38.51	39.00	39.17	39.25	39.30	39.33	39.36	39.37	39.39	39.40	39.41	39.43	39.45	39.46	39.46	39.47	39.48	39.49	39.50
3	17.44	16.04	15.44	15.10	14.88	14.73	14.62	14.54	14.47	14.42	14.34	14.25	14.17	14.12	14.08	14.04	13.99	13.95	13.90
4	12.22	10.65	9.98	9.60	9.36	9.20	9.07	8.98	8.90	8.84	8.75	8.66	8.56	8.51	8.46	8.41	8.36	8.31	8.26
5	10.01	8.43	7.76	7.39	7.15	6.98	6.85	6.76	6.68	6.62	6.52	6.43	6.33	6.28	6.23	6.18	6.12	6.07	6.02
6	8.81	7.26	6.60	6.23	5.99	5.82	5.70	5.60	5.52	5.46	5.37	5.27	5.17	5.12	5.07	5.01	4.96	4.90	4.85
7	8.07	6.54	5.89	5.52	5.29	5.12	4.99	4.90	4.82	4.76	4.67	4.57	4.47	4.42	4.36	4.31	4.25	4.20	4.14
8	7.57	6.06	5.42	5.05	4.82	4.65	4.53	4.43	4.36	4.30	4.20	4.10	4.00	3.95	3.89	3.84	3.78	3.73	3.67
9	7.21	5.71	5.08	4.72	4.48	4.32	4.20	4.10	4.03	3.96	3.87	3.77	3.67	3.61	3.56	3.51	3.45	3.39	3.33
10	6.94	5.46	4.83	4.47	4.24	4.07	3.95	3.85	3.78	3.72	3.62	3.52	3.42	3.37	3.31	3.26	3.20	3.14	3.08
11	6.72	5.26	4.63	4.28	4.04	3.88	3.76	3.66	3.59	3.53	3.43	3.33	3.23	3.17	3.12	3.06	3.00	2.94	2.88
12	6.55	5.10	4.47	4.12	3.89	3.73	3.61	3.51	3.44	3.37	3.28	3.18	3.07	3.02	2.96	2.91	2.85	2.79	2.72
13	6.41	4.97	4.35	4.00	3.77	3.60	3.48	3.39	3.31	3.25	3.15	3.05	2.95	2.89	2.84	2.78	2.72	2.66	2.60
14	6.30	4.86	4.24	3.89	3.66	3.50	3.38	3.29	3.21	3.15	3.05	2.95	2.84	2.79	2.73	2.67	2.61	2.55	2.49
15	6.20	4.77	4.15	3.80	3.58	3.41	3.29	3.20	3.12	3.06	2.96	2.86	2.76	2.70	2.64	2.59	2.52	2.46	2.40
16	6.12	4.69	4.08	3.73	3.50	3.34	3.22	3.12	3.05	2.99	2.89	2.79	2.68	2.63	2.57	2.51	2.45	2.38	2.32
17	6.04	4.62	4.01	3.66	3.44	3.28	3.16	3.06	2.98	2.92	2.82	2.72	2.62	2.56	2.50	2.44	2.38	2.32	2.25
18	5.98	4.56	3.95	3.61	3.38	3.22	3.10	3.01	2.93	2.87	2.77	2.67	2.56	2.50	2.44	2.38	2.32	2.26	2.19
19	5.92	4.51	3.90	3.56	3.33	3.17	3.05	2.96	2.88	2.82	2.72	2.62	2.51	2.45	2.39	2.33	2.27	2.20	2.13
20	5.87	4.46	3.86	3.51	3.29	3.13	3.01	2.91	2.84	2.77	2.68	2.57	2.46	2.41	2.35	2.29	2.22	2.16	2.09
21	5.83	4.42	3.82	3.48	3.25	3.09	2.97	2.87	2.80	2.73	2.64	2.53	2.42	2.37	2.31	2.25	2.18	2.11	2.04
22	5.79	4.38	3.78	3.44	3.22	3.05	2.93	2.84	2.76	2.70	2.60	2.50	2.39	2.33	2.27	2.21	2.14	2.08	2.00
23	5.75	4.35	3.75	3.41	3.18	3.02	2.90	2.81	2.73	2.67	2.57	2.47	2.36	2.30	2.24	2.18	2.11	2.04	1.97
24	5.72	4.32	3.72	3.38	3.15	2.99	2.87	2.78	2.70	2.64	2.54	2.44	2.33	2.27	2.21	2.15	2.08	2.01	1.94
25	5.69	4.29	3.69	3.35	3.13	2.97	2.85	2.75	2.68	2.61	2.51	2.41	2.30	2.24	2.18	2.12	2.05	1.98	1.91
26	5.66	4.27	3.67	3.33	3.10	2.94	2.82	2.73	2.65	2.59	2.49	2.39	2.28	2.22	2.16	2.09	2.03	1.95	1.88
27	5.63	4.24	3.65	3.31	3.08	2.92	2.80	2.71	2.63	2.57	2.47	2.36	2.25	2.19	2.13	2.07	2.00	1.93	1.85
28	5.61	4.22	3.63	3.29	3.06	2.90	2.78	2.69	2.61	2.55	2.45	2.34	2.23	2.17	2.11	2.05	1.98	1.91	1.83
29	5.59	4.20	1.61	3.27	3.04	2.88	2.76	2.67	2.59	2.53	2.43	2.32	2.21	2.15	2.09	2.03	1.96	1.89	1.81
30	5.57	4.18	3.59	3.25	3.03	2.87	2.75	2.65	2.57	2.51	2.41	2.31	2.20	2.14	2.07	2.01	1.94	1.87	1.79
40	5.42	4.05	3.46	3.13	2.90	2.74	2.62	2.53	2.45	2.39	2.29	2.18	2.07	2.01	1.94	1.88	1.80	1.72	1.64
60	5.29	3.93	3.34	3.01	2.79	2.63	2.51	2.41	2.33	2.27	2.17	2.06	1.94	1.88	1.82	1.74	1.67	1.58	1.48
120	5.15	3.80	3.23	2.89	2.67	2.52	2.39	2.30	2.22	2.16	2.05	1.94	1.82	1.76	1.69	1.61	1.53	1.43	1.31

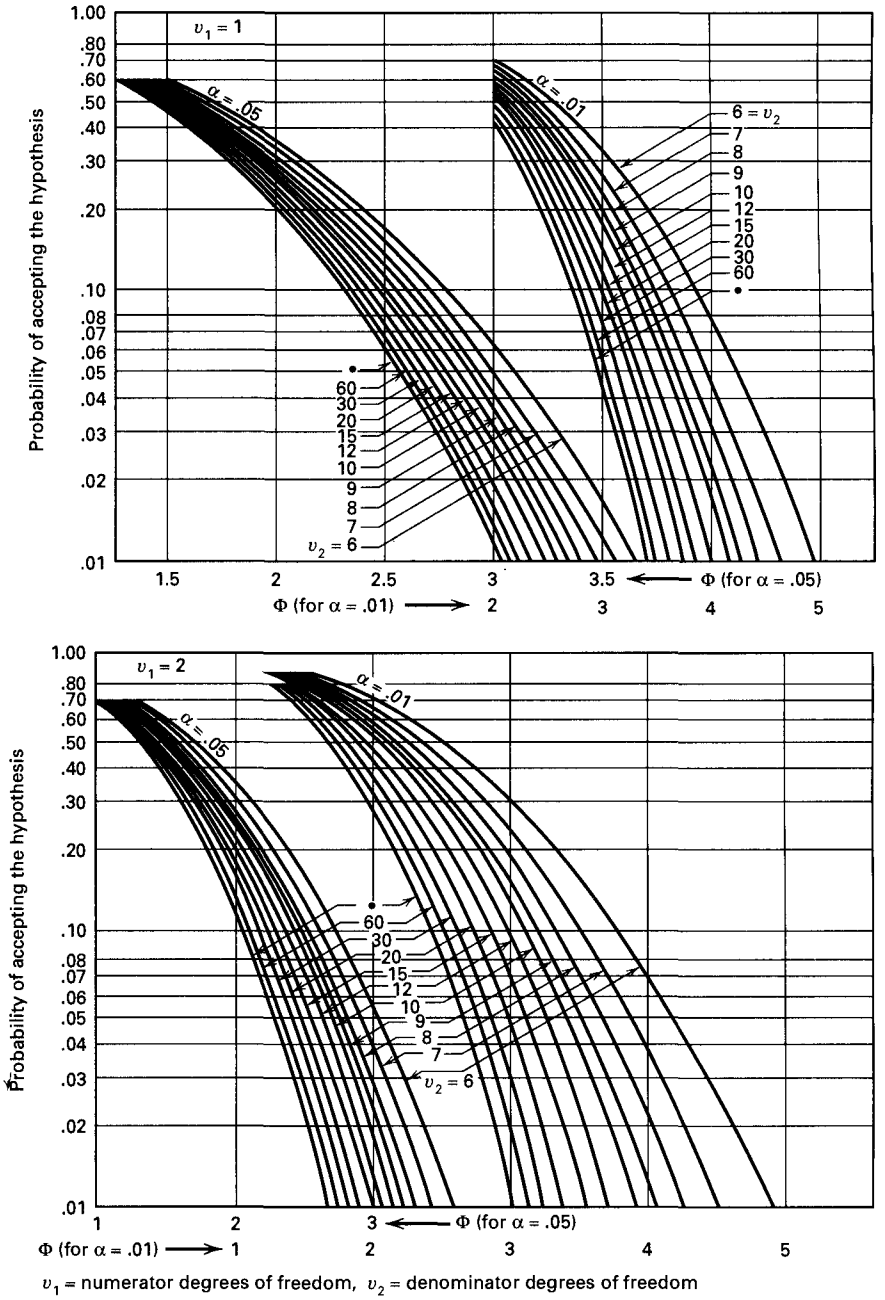
Degrees of Freedom for the Denominator (ν_2)

Degrees of Freedom for the Numerator (ν_1)

ν_2 \ ν_1	1	2	3	4	5	6	7	8	9	10	12	15	20	24	30	40	60	120	∞
1	4052	4999.5	5403	5625	5764	5859	5928	5982	6022	6056	6106	6157	6209	6235	6261	6287	6313	6339	6366
2	98.50	99.00	99.17	99.25	99.30	99.33	99.36	99.37	99.39	99.40	99.42	99.43	99.45	99.46	99.47	99.47	99.48	99.49	99.50
3	34.12	30.82	29.46	28.71	28.24	27.91	27.67	27.49	27.35	27.23	27.05	26.87	26.69	26.00	26.50	26.41	26.32	26.22	26.13
4	21.20	18.00	16.69	15.98	15.52	15.21	14.98	14.80	14.66	14.55	14.37	14.20	14.02	13.93	13.84	13.75	13.65	13.56	13.46
5	16.26	13.27	12.06	11.39	10.97	10.67	10.46	10.29	10.16	10.05	9.89	9.72	9.55	9.47	9.38	9.29	9.20	9.11	9.02
6	13.75	10.92	9.78	9.15	8.75	8.47	8.26	8.10	7.98	7.87	7.72	7.56	7.40	7.31	7.23	7.14	7.06	6.97	6.88
7	12.25	9.55	8.45	7.85	7.46	7.19	6.99	6.84	6.72	6.62	6.47	6.31	6.16	6.07	5.99	5.91	5.82	5.74	5.65
8	11.26	8.65	7.59	7.01	6.63	6.37	6.18	6.03	5.91	5.81	5.67	5.52	5.36	5.28	5.20	5.12	5.03	4.95	4.86
9	10.56	8.02	6.99	6.42	6.06	5.80	5.61	5.47	5.35	5.26	5.11	4.96	4.81	4.73	4.65	4.57	4.48	4.40	4.31
10	10.04	7.56	6.55	5.99	5.64	5.39	5.20	5.06	4.94	4.85	4.71	4.56	4.41	4.33	4.25	4.17	4.08	4.00	3.91
11	9.65	7.21	6.22	5.67	5.32	5.07	4.89	4.74	4.63	4.54	4.40	4.25	4.10	4.02	3.94	3.86	3.78	3.69	3.60
12	9.33	6.93	5.95	5.41	5.06	4.82	4.64	4.50	4.39	4.30	4.16	4.01	3.86	3.78	3.70	3.62	3.54	3.45	3.36
13	9.07	6.70	5.74	5.21	4.86	4.62	4.44	4.30	4.19	4.10	3.96	3.82	3.66	3.59	3.51	3.43	3.34	3.25	3.17
14	8.86	6.51	5.56	5.04	4.69	4.46	4.28	4.14	4.03	3.94	3.80	3.66	3.51	3.43	3.35	3.27	3.18	3.09	3.00
15	8.68	6.36	5.42	4.89	4.56	4.32	4.14	4.00	3.89	3.80	3.67	3.52	3.37	3.29	3.21	3.13	3.05	2.96	2.87
16	8.53	6.23	5.29	4.77	4.44	4.20	4.03	3.89	3.78	3.69	3.55	3.41	3.26	3.18	3.10	3.02	2.93	2.84	2.75
17	8.40	6.11	5.18	4.67	4.34	4.10	3.93	3.79	3.68	3.59	3.46	3.31	3.16	3.08	3.00	2.92	2.83	2.75	2.65
18	8.29	6.01	5.09	4.58	4.25	4.01	3.84	3.71	3.60	3.51	3.37	3.23	3.08	3.00	2.92	2.84	2.75	2.66	2.57
19	8.18	5.93	5.01	4.50	4.17	3.94	3.77	3.63	3.52	3.43	3.30	3.15	3.00	2.92	2.84	2.76	2.67	2.58	2.49
20	8.10	5.85	4.94	4.43	4.10	3.87	3.70	3.56	3.46	3.37	3.23	3.09	2.94	2.86	2.78	2.69	2.61	2.52	2.42
21	8.02	5.78	4.87	4.37	4.04	3.81	3.64	3.51	3.40	3.31	3.17	3.03	2.88	2.80	2.72	2.64	2.55	2.46	2.36
22	7.95	5.72	4.82	4.31	3.99	3.76	3.59	3.45	3.35	3.26	3.12	2.98	2.83	2.75	2.67	2.58	2.50	2.40	2.31
23	7.88	5.66	4.76	4.26	3.94	3.71	3.54	3.41	3.30	3.21	3.07	2.93	2.78	2.70	2.62	2.54	2.45	2.35	2.26
24	7.82	5.61	4.72	4.22	3.90	3.67	3.50	3.36	3.26	3.17	3.03	2.89	2.74	2.66	2.58	2.49	2.40	2.31	2.21
25	7.77	5.57	4.68	4.18	3.85	3.63	3.46	3.32	3.22	3.13	2.99	2.85	2.70	2.62	2.54	2.45	2.36	2.27	2.17
26	7.72	5.53	4.64	4.14	3.82	3.59	3.42	3.29	3.18	3.09	2.96	2.81	2.66	2.58	2.50	2.42	2.33	2.23	2.13
27	7.68	5.49	4.60	4.11	3.78	3.56	3.39	3.26	3.15	3.06	2.93	2.78	2.63	2.55	2.47	2.38	2.29	2.20	2.10
28	7.64	5.45	4.57	4.07	3.75	3.53	3.36	3.23	3.12	3.03	2.90	2.75	2.60	2.52	2.44	2.34	2.26	2.17	2.06
29	7.60	5.42	4.54	4.04	3.73	3.50	3.33	3.20	3.09	3.00	2.87	2.73	2.57	2.49	2.41	2.33	2.23	2.14	2.03
30	7.56	5.39	4.51	4.02	3.70	3.47	3.30	3.17	3.07	2.98	2.84	2.70	2.55	2.47	2.39	2.30	2.21	2.11	2.01
40	7.31	5.18	4.31	3.83	3.51	3.29	3.12	2.99	2.89	2.80	2.66	2.52	2.37	2.29	2.20	2.11	2.02	1.92	1.80
60	7.08	4.98	4.13	3.65	3.34	3.12	2.95	2.82	2.72	2.63	2.50	2.35	2.20	2.12	2.03	1.94	1.84	1.73	1.60
120	6.85	4.79	3.95	3.48	3.17	2.96	2.79	2.66	2.56	2.47	2.34	2.19	2.03	1.95	1.86	1.76	1.66	1.53	1.38

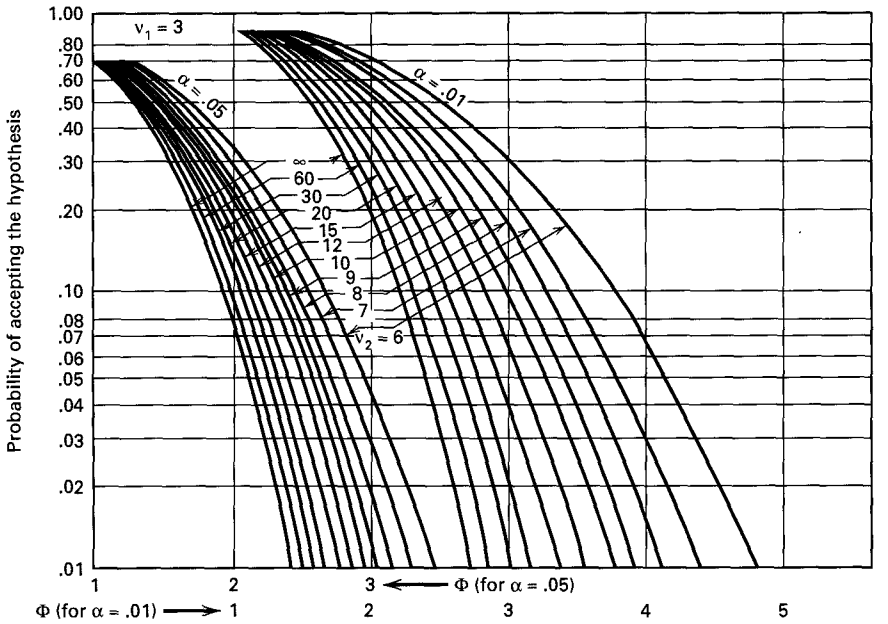
Degrees of Freedom for the Denominator (ν_2)

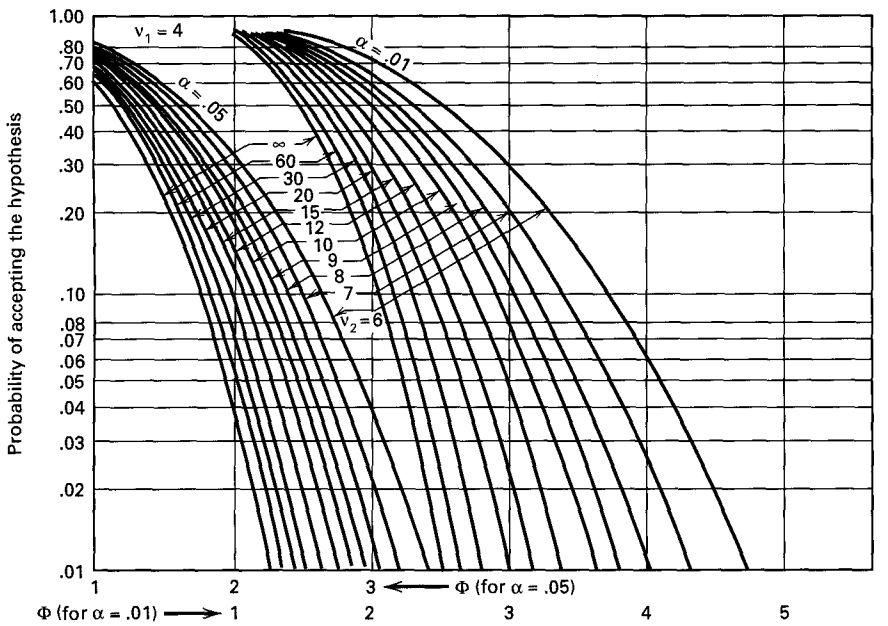
V. Operating Characteristic Curves for the Fixed Effects Model Analysis of Variance[a]


Probability of accepting the hypothesis
$v_1 = 1$
$\alpha = .05$
$\alpha = .01$
$v_2 = 6$
Φ (for α = .01)
Φ (for α = .05)
$v_1 = 2$
v_1 = numerator degrees of freedom, v_2 = denominator degrees of freedom

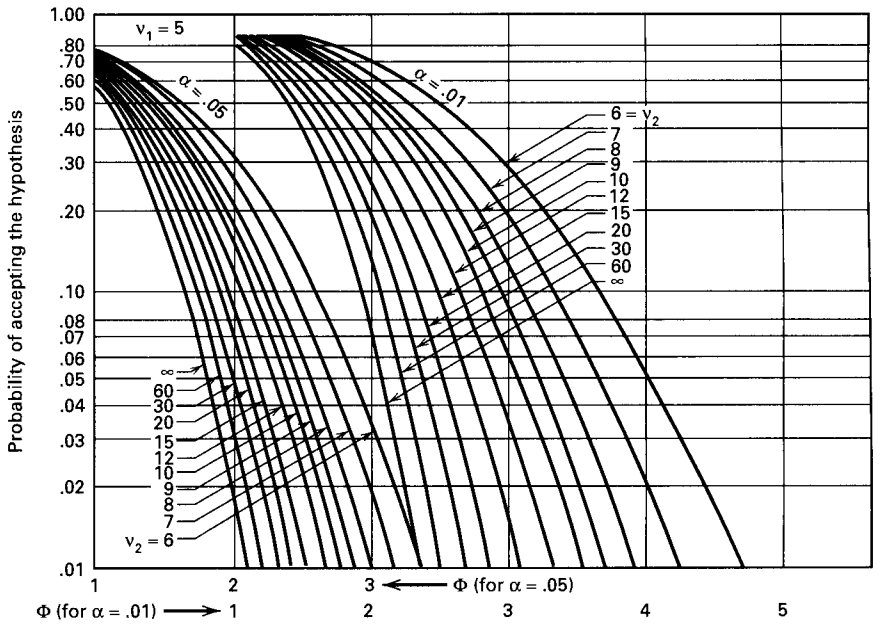
[a] Adapted with permission from *Biometrika Tables for Statisticians*, Vol. 2, by E. S. Pearson and H. O. Hartley, Cambridge University Press, Cambridge, 1972.

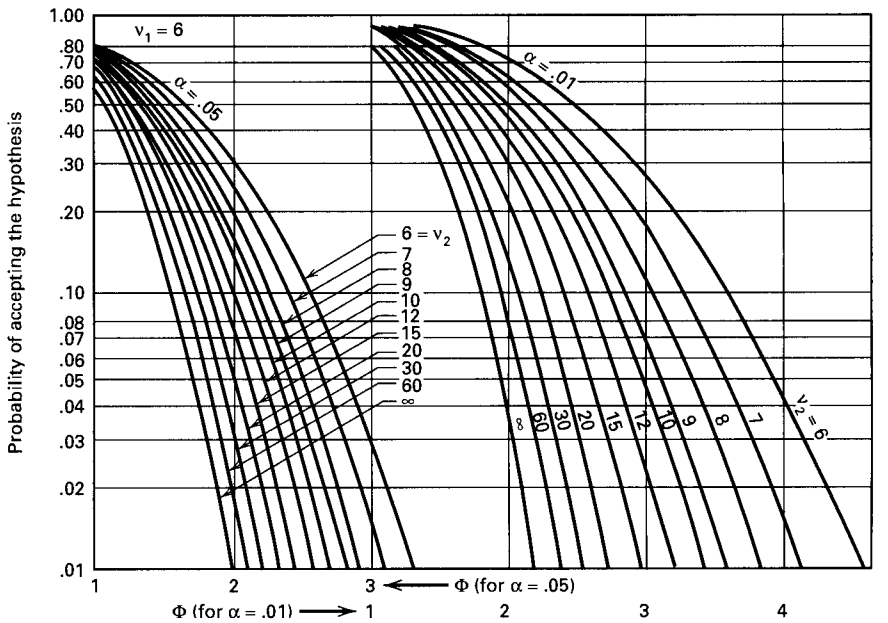
V. Operating Characteristic Curves for the Fixed Effects Model Analysis of Variance (*continued*)



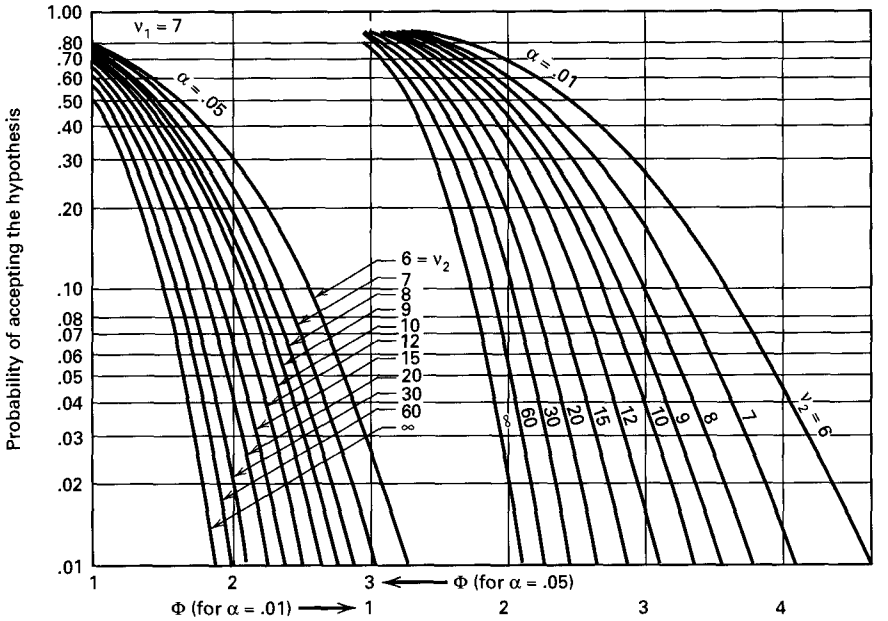


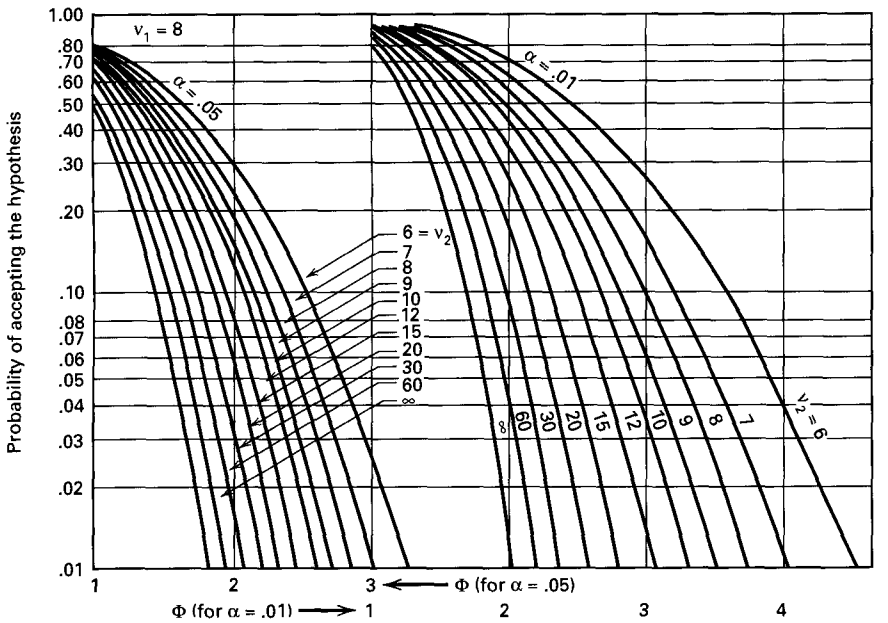
V. Operating Characteristic Curves for the Fixed Effects Model Analysis of Variance (*continued*)



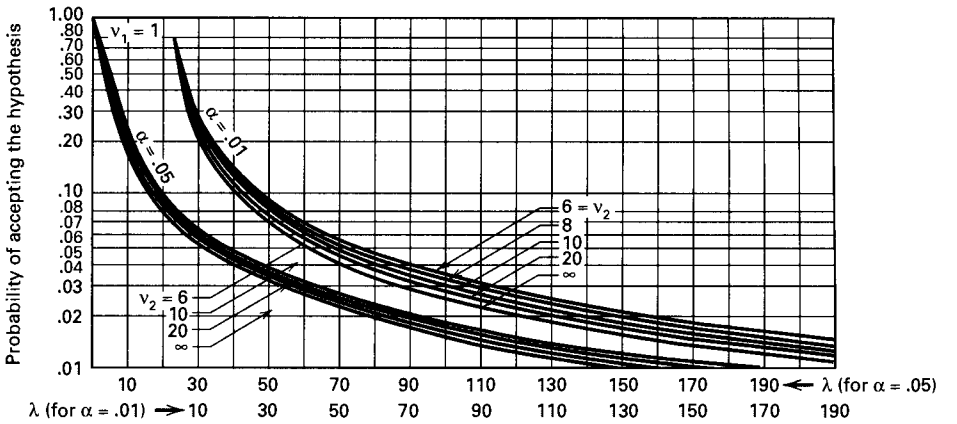


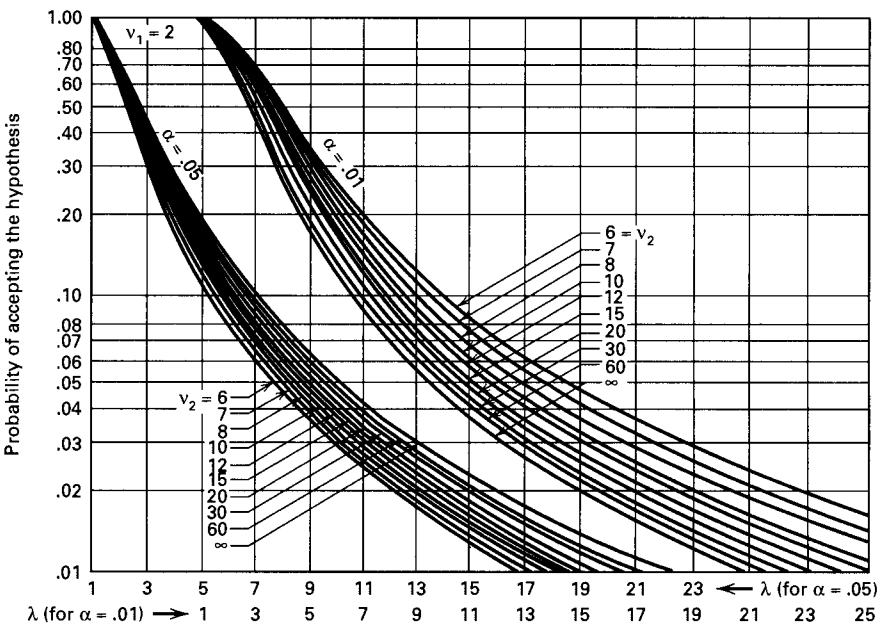
V. Operating Characteristic Curves for the Fixed Effects Model Analysis of Variance (*continued*)





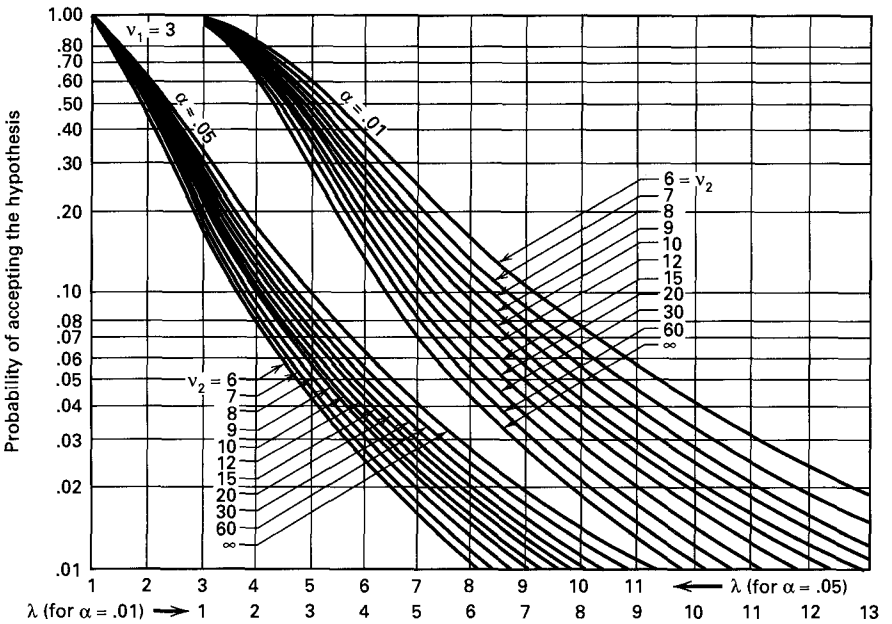
VI. Operating Characteristic Curves for the Random Effects Model Analysis of Variance[a]

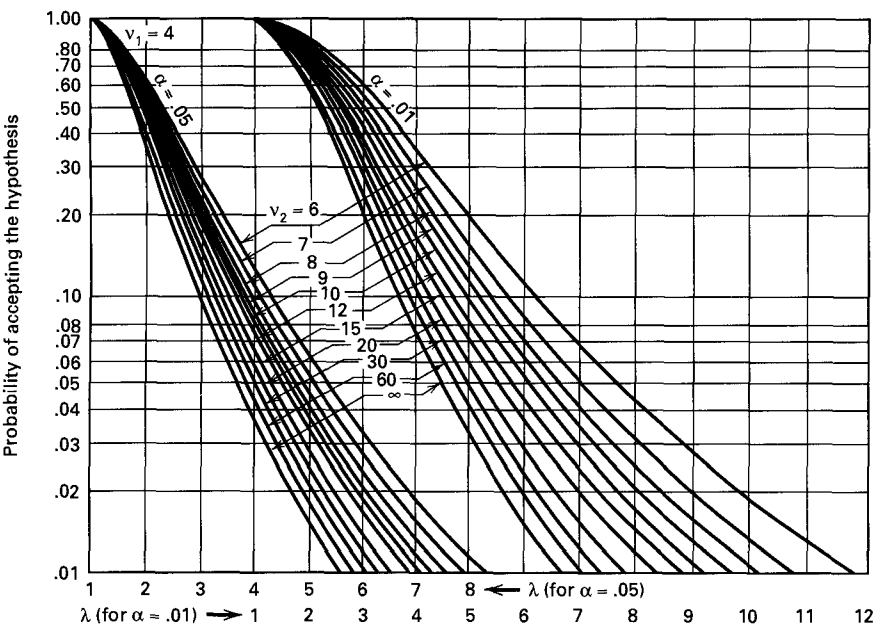




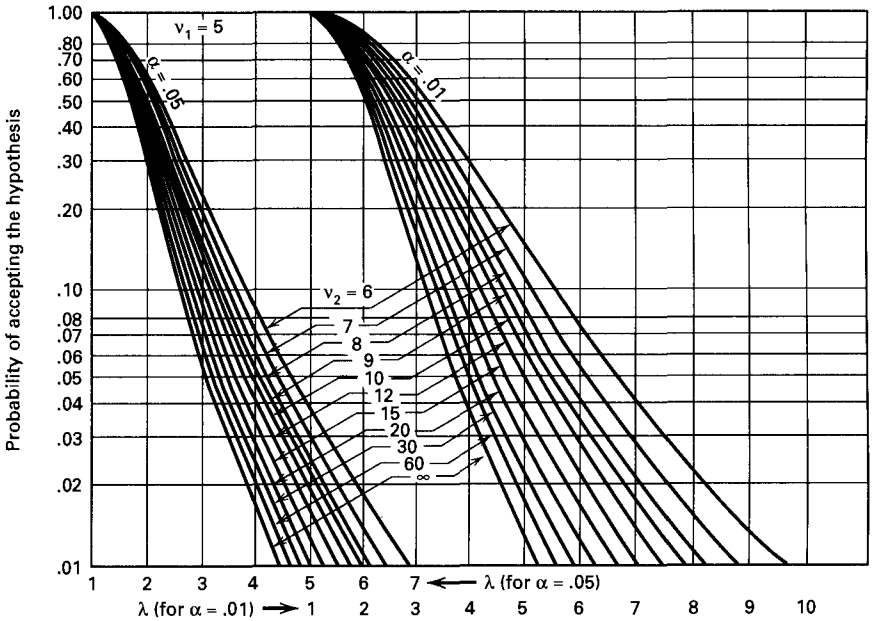
[a] Reproduced with permission from *Engineering Statistics*, 2nd edition, by A. H. Bowker and G. J. Lieberman, Prentice-Hall, Inc., Englewood Cliffs, N.J., 1972.

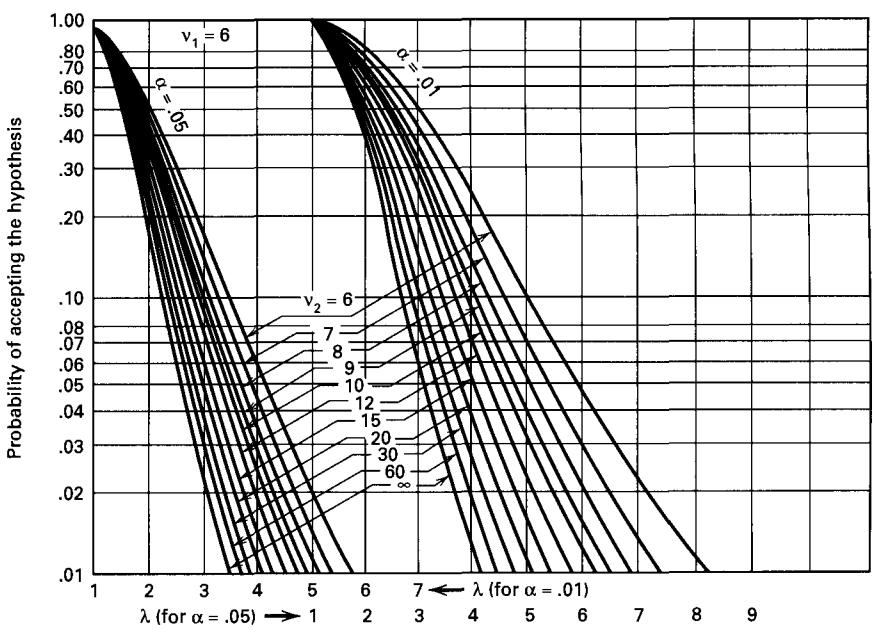
VI. Operating Characteristic Curves for the Random Effects Model Analysis of Variance (*continued*)



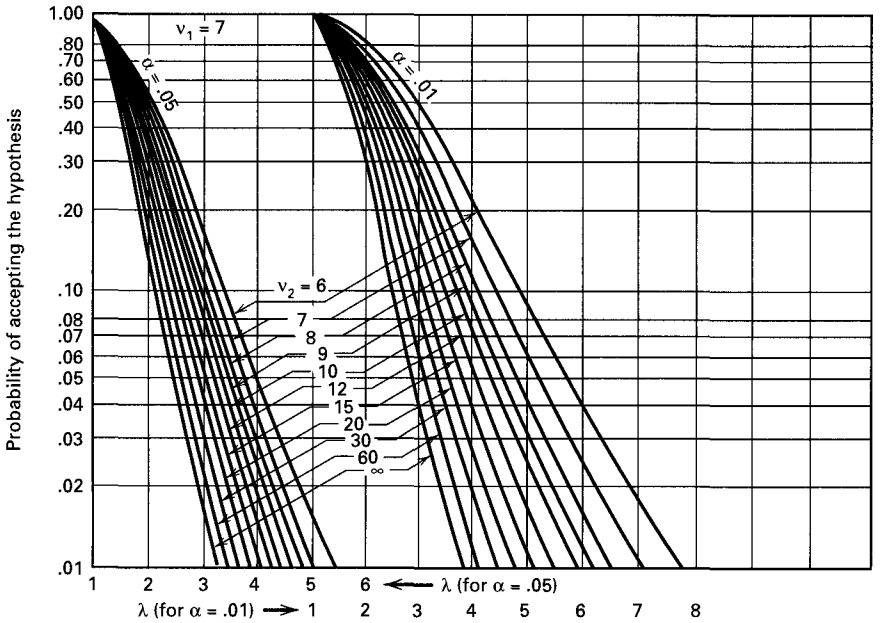


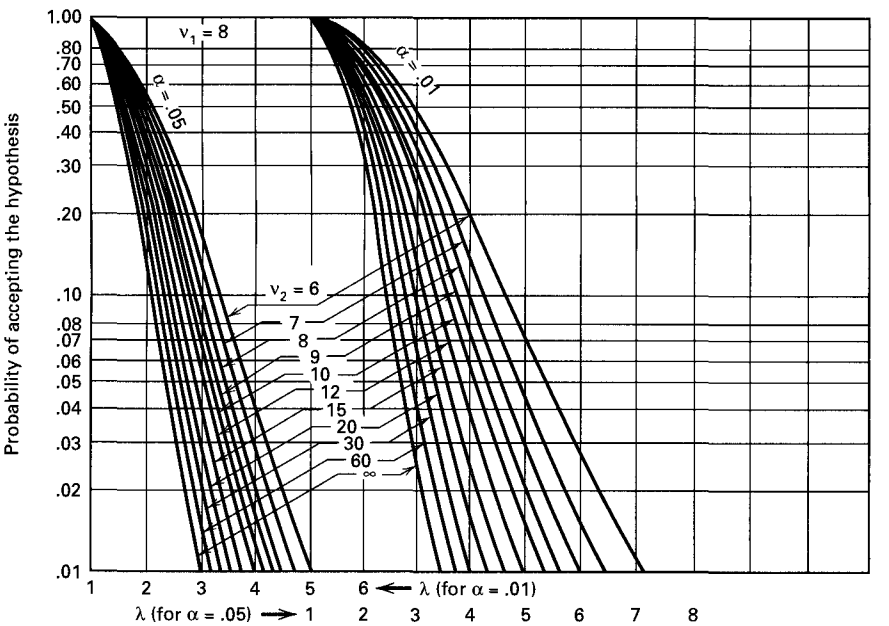
VI. Operating Characteristic Curves for the Random Effects Model Analysis of Variance (*continued*)





VI. Operating Characteristic Curves for the Random Effects Model Analysis of Variance (*continued*)





VII. Significant Ranges for Duncan's Multiple Range Test[a]

$r_{0.01}(p, f)$

	p											
f	2	3	4	5	6	7	8	9	10	20	50	100
1	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
2	14.0	14.0	14.0	14.0	14.0	14.0	14.0	14.0	14.0	14.0	14.0	14.0
3	8.26	8.5	8.6	8.7	8.8	8.9	8.9	9.0	9.0	9.3	9.3	9.3
4	6.51	6.8	6.9	7.0	7.1	7.1	7.2	7.2	7.3	7.5	7.5	7.5
5	5.70	5.96	6.11	6.18	6.26	6.33	6.40	6.44	6.5	6.8	6.8	6.8
6	5.24	5.51	5.65	5.73	5.81	5.88	5.95	6.00	6.0	6.3	6.3	6.3
7	4.95	5.22	5.37	5.45	5.53	5.61	5.69	5.73	5.8	6.0	6.0	6.0
8	4.74	5.00	5.14	5.23	5.32	5.40	5.47	5.51	5.5	5.8	5.8	5.8
9	4.60	4.86	4.99	5.08	5.17	5.25	5.32	5.36	5.4	5.7	5.7	5.7
10	4.48	4.73	4.88	4.96	5.06	5.13	5.20	5.24	5.28	5.55	5.55	5.55
11	4.39	4.63	4.77	4.86	4.94	5.01	5.06	5.12	5.15	5.39	5.39	5.39
12	4.32	4.55	4.68	4.76	4.84	4.92	4.96	5.02	5.07	5.26	5.26	5.26
13	4.26	4.48	4.62	4.69	4.74	4.84	4.88	4.94	4.98	5.15	5.15	5.15
14	4.21	4.42	4.55	4.63	4.70	4.78	4.83	4.87	4.91	5.07	5.07	5.07
15	4.17	4.37	4.50	4.58	4.64	4.72	4.77	4.81	4.84	5.00	5.00	5.00
16	4.13	4.34	4.45	4.54	4.60	4.67	4.72	4.76	4.79	4.94	4.94	4.94
17	4.10	4.30	4.41	4.50	4.56	4.63	4.68	4.73	4.75	4.89	4.89	4.89
18	4.07	4.27	4.38	4.46	4.53	4.59	4.64	4.68	4.71	4.85	4.85	4.85
19	4.05	4.24	4.35	4.43	4.50	4.56	4.61	4.64	4.67	4.82	4.82	4.82
20	4.02	4.22	4.33	4.40	4.47	4.53	4.58	4.61	4.65	4.79	4.79	4.79
30	3.89	4.06	4.16	4.22	4.32	4.36	4.41	4.45	4.48	4.65	4.71	4.71
40	3.82	3.99	4.10	4.17	4.24	4.30	4.34	4.37	4.41	4.59	4.69	4.69
60	3.76	3.92	4.03	4.12	4.17	4.23	4.27	4.31	4.34	4.53	4.66	4.66
100	3.71	3.86	3.98	4.06	4.11	4.17	4.21	4.25	4.29	4.48	4.64	4.65
∞	3.64	3.80	3.90	3.98	4.04	4.09	4.14	4.17	4.20	4.41	4.60	4.68

f = degrees of freedom.

[a] Reproduced with permission from "Multiple Range and Multiple F Tests," by D. B. Duncan, *Biometrics*, Vol. 1, No. 1, pp. 1–42, 1955.

$r_{0.05}(p, f)$

	p											
f	2	3	4	5	6	7	8	9	10	20	50	100
1	18.0	18.0	18.0	18.0	18.0	18.0	18.0	18.0	18.0	18.0	18.0	18.0
2	6.09	6.09	6.09	6.09	6.09	6.09	6.09	6.09	6.09	6.09	6.09	6.09
3	4.50	4.50	4.50	4.50	4.50	4.50	4.50	4.50	4.50	4.50	4.50	4.50
4	3.93	4.01	4.02	4.02	4.02	4.02	4.02	4.02	4.02	4.02	4.02	4.02
5	3.64	3.74	3.79	3.83	3.83	3.83	3.83	3.83	3.83	3.83	3.83	3.83
6	3.46	3.58	3.64	3.68	3.68	3.68	3.68	3.68	3.68	3.68	3.68	3.68
7	3.35	3.47	3.54	3.58	3.60	3.61	3.61	3.61	3.61	3.61	3.61	3.61
8	3.26	3.39	3.47	3.52	3.55	3.56	3.56	3.56	3.56	3.56	3.56	3.56
9	3.20	3.34	3.41	3.47	3.50	3.52	3.52	3.52	3.52	3.52	3.52	3.52
10	3.15	3.30	3.37	3.43	3.46	3.47	3.47	3.47	3.47	3.48	3.48	3.48
11	3.11	3.27	3.35	3.39	3.43	3.44	3.45	3.46	3.46	3.48	3.48	3.48
12	3.08	3.23	3.33	3.36	3.40	3.42	3.44	3.44	3.46	3.48	3.48	3.48
13	3.06	3.21	3.30	3.35	3.38	3.41	3.42	3.44	3.45	3.47	3.47	3.47
14	3.03	3.18	3.27	3.33	3.37	3.39	3.41	3.42	3.44	3.47	3.47	3.47
15	3.01	3.16	3.25	3.31	3.36	3.38	3.40	3.42	3.43	3.47	3.47	3.47
16	3.00	3.15	3.23	3.30	3.34	3.37	3.39	3.41	3.43	3.47	3.47	3.47
17	2.98	3.13	3.22	3.28	3.33	3.36	3.38	3.40	3.42	3.47	3.47	3.47
18	2.97	3.12	3.21	3.27	3.32	3.35	3.37	3.39	3.41	3.47	3.47	3.47
19	2.96	3.11	3.19	3.26	3.31	3.35	3.37	3.39	3.41	3.47	3.47	3.47
20	2.95	3.10	3.18	3.25	3.30	3.34	3.36	3.38	3.40	3.47	3.47	3.47
30	2.89	3.04	3.12	3.20	3.25	3.29	3.32	3.35	3.37	3.47	3.47	3.47
40	2.86	3.01	3.10	3.17	3.22	3.27	3.30	3.33	3.35	3.47	3.47	3.47
60	2.83	2.98	3.08	3.14	3.20	3.24	3.28	3.31	3.33	3.47	3.48	3.48
100	2.80	2.95	3.05	3.12	3.18	3.22	3.26	3.29	3.32	3.47	3.53	3.53
∞	2.77	2.92	3.02	3.09	3.15	3.19	3.23	3.26	3.29	3.47	3.61	3.67

	p																		
f	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	90.0	135	164	186	202	216	227	237	246	253	260	266	272	272	282	286	290	294	298
2	14.0	19.0	22.3	24.7	26.6	28.2	29.5	30.7	31.7	32.6	33.4	31.4	34.8	35.4	36.0	36.5	37.0	37.5	37.9
3	8.26	10.6	12.2	13.3	14.2	15.0	15.6	16.2	16.7	17.1	17.5	17.9	18.2	18.5	18.8	19.1	19.3	19.5	19.8
4	6.51	8.12	9.17	9.96	10.6	11.1	11.5	11.9	12.3	12.6	12.8	13.1	13.3	13.5	13.7	13.9	14.1	14.2	14.4
5	5.70	6.97	7.80	8.42	8.91	9.32	9.67	9.97	10.24	10.48	10.70	10.89	11.08	11.24	11.40	11.55	11.68	11.81	11.93
6	5.24	6.33	7.03	7.56	7.97	8.32	8.61	8.87	9.10	9.30	9.49	9.65	9.81	9.95	10.08	10.21	10.32	10.43	10.54
7	4.95	5.92	6.54	7.01	7.37	7.68	7.94	8.17	8.37	8.55	8.71	8.86	9.00	9.12	9.24	9.35	9.46	9.55	9.65
8	4.74	5.63	6.20	6.63	6.96	7.24	7.47	7.68	7.87	8.03	8.18	8.31	8.44	8.55	8.66	8.76	8.85	8.94	9.03
9	4.60	5.43	5.96	6.35	6.66	6.91	7.13	7.32	7.49	7.65	7.78	7.91	8.03	8.13	8.23	8.32	8.41	8.49	8.57
10	4.48	5.27	5.77	6.14	6.43	6.67	6.87	7.05	7.21	7.36	7.48	7.60	7.71	7.81	7.91	7.99	8.07	8.15	8.22
11	4.39	5.14	5.62	5.97	6.25	6.48	6.67	6.84	6.99	7.13	7.25	7.36	7.46	7.56	7.65	7.73	7.81	7.88	7.95
12	4.32	5.04	5.50	5.84	6.10	6.32	6.51	6.67	6.81	6.94	7.06	7.17	7.26	7.36	7.44	7.52	7.59	7.66	7.73
13	4.26	4.96	5.40	5.73	5.98	6.19	6.37	6.53	6.67	6.79	6.90	7.01	7.10	7.19	7.27	7.34	7.42	7.48	7.55
14	4.21	4.89	5.32	5.63	5.88	6.08	6.26	6.41	6.54	6.66	6.77	6.87	6.96	7.05	7.12	7.20	7.27	7.33	7.39
15	4.17	4.83	5.25	5.56	5.80	5.99	6.16	6.31	6.44	6.55	6.66	6.76	6.84	6.93	7.00	7.07	7.14	7.20	7.26
16	4.13	4.78	5.19	5.49	5.72	5.92	6.08	6.22	6.35	6.46	6.56	6.66	6.74	6.82	6.90	6.97	7.03	7.09	7.15
17	4.10	4.74	5.14	5.43	5.66	5.85	6.01	6.15	6.27	6.38	6.48	6.57	6.66	6.73	6.80	6.87	6.94	7.00	7.05
18	4.07	4.70	5.09	5.38	5.60	5.79	5.94	6.08	6.20	6.31	6.41	6.50	6.58	6.65	6.72	6.79	6.85	6.91	6.96
19	4.05	4.67	5.05	5.33	5.55	5.73	5.89	6.02	6.14	6.25	6.34	6.43	6.51	6.58	6.65	6.72	6.78	6.84	6.89
20	4.02	4.64	5.02	5.29	5.51	5.69	5.84	5.97	6.09	6.19	6.29	6.37	6.45	6.52	6.59	6.65	6.71	6.76	6.82
24	3.96	4.54	4.91	5.17	5.37	5.54	5.69	5.81	5.92	6.02	6.11	6.19	6.26	6.33	6.39	6.45	6.51	6.56	6.61
30	3.89	4.45	4.80	5.05	5.24	5.40	5.54	5.65	5.76	5.85	5.93	6.01	6.08	6.14	6.20	6.26	6.31	6.36	6.41
40	3.82	4.37	4.70	4.93	5.11	5.27	5.39	5.50	5.60	5.69	5.77	5.84	5.90	5.96	6.02	6.07	6.12	6.17	6.21
60	3.76	4.28	4.60	4.82	4.99	5.13	5.25	5.36	5.45	5.53	5.60	5.67	5.73	5.79	5.84	5.89	5.93	5.98	6.02
120	3.70	4.20	4.50	4.71	4.87	5.01	5.12	5.21	5.30	5.38	5.44	5.51	5.56	5.61	5.66	5.71	5.75	5.79	5.83
∞	3.64	4.12	4.40	4.60	4.76	4.88	4.99	5.08	5.16	5.23	5.29	5.35	5.40	5.45	5.49	5.54	5.57	5.61	5.65

f = degress of freedom.

[a] From J. M. May, "Extended and Corrected Tables of the Upper Percentage Points of the Studentized Range," *Biometrika*, Vol. 39, pp. 192–193, 1952. Reproduced by permission of the

$q_{0.05}(p, f)$

	p																		
f	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	18.1	26.7	32.8	37.2	40.5	43.1	45.4	47.3	49.1	50.6	51.9	53.2	54.3	55.4	56.3	57.2	58.0	58.8	59.6
2	6.09	8.28	9.80	10.89	11.73	12.43	13.03	13.54	13.99	14.39	14.75	15.08	15.38	15.65	15.91	16.14	16.36	16.57	16.77
3	4.50	5.88	6.83	7.51	8.04	8.47	8.85	9.18	9.46	9.72	9.95	10.16	10.35	10.52	10.69	10.84	10.98	11.12	11.24
4	3.93	5.00	5.76	6.31	6.73	7.06	7.35	7.60	7.83	8.03	8.21	8.37	8.52	8.67	8.80	8.92	9.03	9.14	9.24
5	3.64	4.60	5.22	5.67	6.03	6.33	6.58	6.80	6.99	7.17	7.32	7.47	7.60	7.72	7.83	7.93	8.03	8.12	8.21
6	3.46	4.34	4.90	5.31	5.63	5.89	6.12	6.32	6.49	6.65	6.79	6.92	7.04	7.14	7.24	7.34	7.43	7.51	7.59
7	3.34	4.16	4.68	5.06	5.35	5.59	5.80	5.99	6.15	6.29	6.42	6.54	6.65	6.75	6.84	6.93	7.01	7.08	7.16
8	3.26	4.04	4.53	4.89	5.17	5.40	5.60	5.77	5.92	6.05	6.18	6.29	6.39	6.48	6.57	6.65	6.73	6.80	6.87
9	3.20	3.95	4.42	4.76	5.02	5.24	5.43	5.60	5.74	5.87	5.98	6.09	6.19	6.28	6.36	6.44	6.51	6.58	6.65
10	3.15	3.88	4.33	4.66	4.91	5.12	5.30	5.46	5.60	5.72	5.83	5.93	6.03	6.12	6.20	6.27	6.34	6.41	6.47
11	3.11	3.82	4.26	4.58	4.82	5.03	5.20	5.35	5.49	5.61	5.71	5.81	5.90	5.98	6.06	6.14	6.20	6.27	6.33
12	3.08	3.77	4.20	4.51	4.75	4.95	5.12	5.27	5.40	5.51	5.61	5.71	5.80	5.88	5.95	6.02	6.09	6.15	6.21
13	3.06	3.73	4.15	4.46	4.69	4.88	5.05	5.19	5.32	5.43	5.53	5.63	5.71	5.79	5.86	5.93	6.00	6.06	6.11
14	3.03	3.70	4.11	4.41	4.64	4.83	4.99	5.13	5.25	5.36	5.46	5.56	5.64	5.72	5.79	5.86	5.92	5.98	6.03
15	3.01	3.67	4.08	4.37	4.59	4.78	4.94	5.08	5.20	5.31	5.40	5.49	5.57	5.65	5.72	5.79	5.85	5.91	5.96
16	3.00	3.65	4.05	4.34	4.56	4.74	4.90	5.03	5.15	5.26	5.35	5.44	5.52	5.59	5.66	5.73	5.79	5.84	5.90
17	2.98	3.62	4.02	4.31	4.52	4.70	4.86	4.99	5.11	5.21	5.31	5.39	5.47	5.55	5.61	5.68	5.74	5.79	5.84
18	2.97	3.61	4.00	4.28	4.49	4.67	4.83	4.96	5.07	5.17	5.27	5.35	5.43	5.50	5.57	5.63	5.69	5.74	5.79
19	2.96	3.59	3.98	4.26	4.47	4.64	4.79	4.92	5.04	5.14	5.23	5.32	5.39	5.46	5.53	5.59	5.65	5.70	5.75
20	2.95	3.58	3.96	4.24	4.45	4.62	4.77	4.90	5.01	5.11	5.20	5.28	5.36	5.43	5.50	5.56	5.61	5.66	5.71
24	2.92	3.53	3.90	4.17	4.37	4.54	4.68	4.81	4.92	5.01	5.10	5.18	5.25	5.32	5.38	5.44	5.50	5.55	5.59
30	2.89	3.48	3.84	4.11	4.30	4.46	4.60	4.72	4.83	4.92	5.00	5.08	5.15	5.21	5.27	5.33	5.38	5.43	5.48
40	2.86	3.44	3.79	4.04	4.23	4.39	4.52	4.63	4.74	4.82	4.90	4.98	5.05	5.11	5.17	5.22	5.27	5.32	5.36
60	2.83	3.40	3.74	3.98	4.16	4.31	4.44	4.55	4.65	4.73	4.81	4.88	4.94	5.00	5.06	5.11	5.15	5.20	5.24
120	2.80	3.36	3.69	3.92	4.10	4.24	4.36	4.47	4.56	4.64	4.71	4.78	4.84	4.90	4.95	5.00	5.04	5.09	5.13
∞	2.77	3.32	3.63	3.86	4.03	4.17	4.29	4.39	4.47	4.55	4.62	4.68	4.74	4.80	4.84	4.98	4.93	4.97	5.01

IX. Critical Values for Dunnett's Test for Comparing Treatments with a Control[a]
$d_{0.05}(a-1, f)$
Two-Sided Comparisons

	$a-1$ = Number of Treatment Means (excluding control)								
f	1	2	3	4	5	6	7	8	9
5	2.57	3.03	3.29	3.48	3.62	3.73	3.82	3.90	3.97
6	2.45	2.86	3.10	3.26	3.39	3.49	3.57	3.64	3.71
7	2.36	2.75	2.97	3.12	3.24	3.33	3.41	3.47	3.53
8	2.31	2.67	2.88	3.02	3.13	3.22	3.29	3.35	3.41
9	2.26	2.61	2.81	2.95	3.05	3.14	3.20	3.26	3.32
10	2.23	2.57	2.76	2.89	2.99	3.07	3.14	3.19	3.24
11	2.20	2.53	2.72	2.84	2.94	3.02	3.08	3.14	3.19
12	2.18	2.50	2.68	2.81	2.90	2.98	3.04	3.09	3.14
13	2.16	2.48	2.65	2.78	2.87	2.94	3.00	3.06	3.10
14	2.14	2.46	2.63	2.75	2.84	2.91	2.97	3.02	3.07
15	2.13	2.44	2.61	2.73	2.82	2.89	2.95	3.00	3.04
16	2.12	2.42	2.59	2.71	2.80	2.87	2.92	2.97	3.02
17	2.11	2.41	2.58	2.69	2.78	2.85	2.90	2.95	3.00
18	2.10	2.40	2.56	2.68	2.76	2.83	2.89	2.94	2.98
19	2.09	2.39	2.55	2.66	2.75	2.81	2.87	2.92	2.96
20	2.09	2.38	2.54	2.65	2.73	2.80	2.86	2.90	2.95
24	2.06	2.35	2.51	2.61	2.70	2.76	2.81	2.86	2.90
30	2.04	2.32	2.47	2.58	2.66	2.72	2.77	2.82	2.86
40	2.02	2.29	2.44	2.54	2.62	2.68	2.73	2.77	2.81
60	2.00	2.27	2.41	2.51	2.58	2.64	2.69	2.73	2.77
120	1.98	2.24	2.38	2.47	2.55	2.60	2.65	2.69	2.73
∞	1.96	2.21	2.35	2.44	2.51	2.57	2.61	2.65	2.69

f = degrees of freedom.

[a] Reproduced with permission from C. W. Dunnett, "New Tables for Multiple Comparison with a Control," *Biometrics*, Vol. 20, No. 3, 1964, and from C. W. Dunnett, "A Multiple Comparison Procedure for Comparing Several Treatments with a Control," *Journal of the American Statistical Association*, Vol. 50, 1955.

IX. Critical Values for Dunnett's Test for Comparing Treatments with a Control

$d_{0.01}(a-1, f)$

Two-Sided Comparisons (*continued*)

	$a-1$ = Number of Treatment Means (excluding control)								
f	1	2	3	4	5	6	7	8	9
5	4.03	4.63	4.98	5.22	5.41	5.56	5.69	5.80	5.89
6	3.71	4.21	4.51	4.71	4.87	5.00	5.10	5.20	5.28
7	3.50	3.95	4.21	4.39	4.53	4.64	4.74	4.82	4.89
8	3.36	3.77	4.00	4.17	4.29	4.40	4.48	4.56	4.62
9	3.25	3.63	3.85	4.01	4.12	4.22	4.30	4.37	4.43
10	3.17	3.53	3.74	3.88	3.99	4.08	4.16	4.22	4.28
11	3.11	3.45	3.65	3.79	3.89	3.98	4.05	4.11	4.16
12	3.05	3.39	3.58	3.71	3.81	3.89	3.96	4.02	4.07
13	3.01	3.33	3.52	3.65	3.74	3.82	3.89	3.94	3.99
14	2.98	3.29	3.47	3.59	3.69	3.76	3.83	3.88	3.93
15	2.95	3.25	3.43	3.55	3.64	3.71	3.78	3.83	3.88
16	2.92	3.22	3.39	3.51	3.60	3.67	3.73	3.78	3.83
17	2.90	3.19	3.36	3.47	3.56	3.63	3.69	3.74	3.79
18	2.88	3.17	3.33	3.44	3.53	3.60	3.66	3.71	3.75
19	2.86	3.15	3.31	3.42	3.50	3.57	3.63	3.68	3.72
20	2.85	3.13	3.29	3.40	3.48	3.55	3.60	3.65	3.69
24	2.80	3.07	3.22	3.32	3.40	3.47	3.52	3.57	3.61
30	2.75	3.01	3.15	3.25	3.33	3.39	3.44	3.49	3.52
40	2.70	2.95	3.09	3.19	3.26	3.32	3.37	3.41	3.44
60	2.66	2.90	3.03	3.12	3.19	3.25	3.29	3.33	3.37
120	2.62	2.85	2.97	3.06	3.12	3.18	3.22	3.26	3.29
∞	2.58	2.79	2.92	3.00	3.06	3.11	3.15	3.19	3.22

$d_{0.05}(a-1, f)$

One-Sided Comparisons

	$a-1$ = Number of Treatment Means (excluding control)								
f	1	2	3	4	5	6	7	8	9
5	2.02	2.44	2.68	2.85	2.98	3.08	3.16	3.24	3.30
6	1.94	2.34	2.56	2.71	2.83	2.92	3.00	3.07	3.12
7	1.89	2.27	2.48	2.62	2.73	2.82	2.89	2.95	3.01
8	1.86	2.22	2.42	2.55	2.66	2.74	2.81	2.87	2.92
9	1.83	2.18	2.37	2.50	2.60	2.68	2.75	2.81	2.86
10	1.81	2.15	2.34	2.47	2.56	2.64	2.70	2.76	2.81
11	1.80	2.13	2.31	2.44	2.53	2.60	2.67	2.72	2.77
12	1.78	2.11	2.29	2.41	2.50	2.58	2.64	2.69	2.74
13	1.77	2.09	2.27	2.39	2.48	2.55	2.61	2.66	2.71
14	1.76	2.08	2.25	2.37	2.46	2.53	2.59	2.64	2.69
15	1.75	2.07	2.24	2.36	2.44	2.51	2.57	2.62	2.67
16	1.75	2.06	2.23	2.34	2.43	2.50	2.56	2.61	2.65
17	1.74	2.05	2.22	2.33	2.42	2.49	2.54	2.59	2.64
18	1.73	2.04	2.21	2.32	2.41	2.48	2.53	2.58	2.62
19	1.73	2.03	2.20	2.31	2.40	2.47	2.52	2.57	2.61
20	1.72	2.03	2.19	2.30	2.39	2.46	2.51	2.56	2.60
24	1.71	2.01	2.17	2.28	2.36	2.43	2.48	2.53	2.57
30	1.70	1.99	2.15	2.25	2.33	2.40	2.45	2.50	2.54
40	1.68	1.97	2.13	2.23	2.31	2.37	2.42	2.47	2.51
60	1.67	1.95	2.10	2.21	2.28	2.35	2.39	2.44	2.48
120	1.66	1.93	2.08	2.18	2.26	2.32	2.37	2.41	2.45
∞	1.64	1.92	2.06	2.16	2.23	2.29	2.34	2.38	2.42

IX. Critical Values for Dunnett's Test for Comparing Treatments with a Control
$d_{0.01}(a-1, f)$
One-Sided Comparisons (*continued*)

	$a-1$ = Number of Treatment Means (excluding control)								
f	1	2	3	4	5	6	7	8	9
5	3.37	3.90	4.21	4.43	4.60	4.73	4.85	4.94	5.03
6	3.14	3.61	3.88	4.07	4.21	4.33	4.43	4.51	4.59
7	3.00	3.42	3.66	3.83	3.96	4.07	4.15	4.23	4.30
8	2.90	3.29	3.51	3.67	3.79	3.88	3.96	4.03	4.09
9	2.82	3.19	3.40	3.55	3.66	3.75	3.82	3.89	3.94
10	2.76	3.11	3.31	3.45	3.56	3.64	3.71	3.78	3.83
11	2.72	3.06	3.25	3.38	3.48	3.56	3.63	3.69	3.74
12	2.68	3.01	3.19	3.32	3.42	3.50	3.56	3.62	3.67
13	2.65	2.97	3.15	3.27	3.37	3.44	3.51	3.56	3.61
14	2.62	2.94	3.11	3.23	3.32	3.40	3.46	3.51	3.56
15	2.60	2.91	3.08	3.20	3.29	3.36	3.42	3.47	3.52
16	2.58	2.88	3.05	3.17	3.26	3.33	3.39	3.44	3.48
17	2.57	2.86	3.03	3.14	3.23	3.30	3.36	3.41	3.45
18	2.55	2.84	3.01	3.12	3.21	3.27	3.33	3.38	3.42
19	2.54	2.83	2.99	3.10	3.18	3.25	3.31	3.36	3.40
20	2.53	2.81	2.97	3.08	3.17	3.23	3.29	3.34	3.38
24	2.49	2.77	2.92	3.03	3.11	3.17	3.22	3.27	3.31
30	2.46	2.72	2.87	2.97	3.05	3.11	3.16	3.21	3.24
40	2.42	2.68	2.82	2.92	2.99	3.05	3.10	3.14	3.18
60	2.39	2.64	2.78	2.87	2.94	3.00	3.04	3.08	3.12
120	2.36	2.60	2.73	2.82	2.89	2.94	2.99	3.03	3.06
∞	2.33	2.56	2.68	2.77	2.84	2.89	2.93	2.97	3.00

		$n=3$		$n=4$			$n=5$				$n=6$					$n=7$					
	X_j	P_1	P_2	P_1	P_2	P_3	P_1	P_2	P_3	P_4	P_1	P_2	P_3	P_4	P_5	P_1	P_2	P_3	P_4	P_5	P_6
	1	−1	1	−3	1	−1	−2	2	−1	1	−5	5	−5	1	−1	−3	5	−1	3	−1	1
	2	0	−2	−1	−1	3	1	−1	2	−4	−3	−1	7	−3	5	−2	0	1	−7	4	−6
	3	1	1	1	−1	−3	0	−2	0	6	−1	−4	4	2	−10	−1	−3	1	1	−5	15
	4			3	1	1	1	−1	−2	−4	1	−4	−4	2	10	0	−4	0	6	0	−20
	5						2	2	1	1	3	−1	−7	−3	−5	1	−3	−1	1	5	15
	6										5	5	5	1	1	2	0	−1	−7	−4	−6
	7															3	5	1	3	1	1
$\sum_{j=1}^{n} \{P_i(X_j)\}^2$		2	6	20	4	20	10	14	10	70	70	84	180	28	252	28	84	6	154	84	924
	λ	1	3	2	1	$\frac{10}{3}$	1	1	$\frac{5}{6}$	$\frac{35}{12}$	2	$\frac{3}{2}$	$\frac{5}{3}$	$\frac{7}{12}$	$\frac{21}{10}$	1	1	$\frac{1}{6}$	$\frac{7}{12}$	$\frac{7}{20}$	$\frac{77}{60}$

		$n=8$						$n=9$						$n=10$					
	X_j	P_1	P_2	P_3	P_4	P_5	P_6	P_1	P_2	P_3	P_4	P_5	P_6	P_1	P_2	P_3	P_4	P_5	P_6
	1	−7	7	−7	7	−7	1	−4	28	−14	14	−4	4	−9	6	−42	18	−6	3
	2	−5	1	5	−13	23	−5	−3	7	7	−21	11	−17	−7	2	14	−22	14	−11
	3	−3	−3	7	−3	−17	9	−2	−8	13	−11	−4	22	−5	−1	35	−17	−1	10
	4	−1	−5	3	9	−15	−5	−1	−17	9	9	−9	1	−3	−3	31	3	−11	6
	5	1	−5	−3	9	15	−5	0	−20	0	18	0	−20	−1	−4	12	18	−6	−8
	6	3	−3	−7	−3	17	9	1	−17	−9	9	9	1	1	−4	−12	18	6	−8
	7	5	1	−5	−13	−23	−5	2	−8	−13	−11	4	22	3	−3	−31	3	11	6
	8	7	7	7	7	7	1	3	7	−7	−21	−11	−17	5	−1	−35	−17	1	10
	9							4	28	14	14	4	4	7	2	−14	−22	−14	−11
	10													9	6	42	18	6	3
$\sum_{j=1}^{n} \{P_i(X_j)\}^2$		168	168	264	616	2184	264	60	2772	990	2002	468	1980	330	132	8580	2860	780	660
	λ	2	1	$\frac{2}{3}$	$\frac{7}{12}$	$\frac{7}{10}$	$\frac{11}{60}$	1	3	$\frac{5}{6}$	$\frac{7}{12}$	$\frac{3}{20}$	$\frac{11}{60}$	2	$\frac{1}{2}$	$\frac{5}{3}$	$\frac{5}{12}$	$\frac{1}{10}$	$\frac{11}{240}$

[a] Adapted with permission from *Biometrika Tables for Statisticians*, Vol. 1, 3rd edition by E. S. Pearson and H. O. Hartley, Cambridge University Press, Cambridge, 1966.

XI. Random Numbers[a]

10480	15011	01536	02011	87647	91646	69179	14194	62590
22368	46573	25595	85393	30995	89198	27982	53402	93965
24130	48360	22527	97265	76393	64809	15179	24830	49340
42167	93093	06243	61680	07856	16376	39440	53537	71341
37570	39975	81837	16656	06121	91782	60468	81305	49684
77921	06907	11008	42751	27756	53498	18602	70659	90655
99562	72905	56420	69994	98872	31016	71194	18738	44013
96301	91977	05463	07972	18876	20922	94595	56869	69014
89579	14342	63661	10281	17453	18103	57740	84378	25331
85475	36857	53342	53988	53060	59533	38867	62300	08158
28918	69578	88231	33276	70997	79936	56865	05859	90106
63553	40961	48235	03427	49626	69445	18663	72695	52180
09429	93969	52636	92737	88974	33488	36320	17617	30015
10365	61129	87529	85689	48237	52267	67689	93394	01511
07119	97336	71048	08178	77233	13976	47564	81056	97735
51085	12765	51821	51259	77452	16308	60756	92144	49442
02368	21382	52404	60268	89368	19885	55322	44819	01188
01011	54092	33362	94904	31273	04146	18594	29852	71585
52162	53916	46369	58586	23216	14513	83149	98736	23495
07056	97628	33787	09998	42698	06691	76988	13602	51851
48663	91245	85828	14346	09172	30168	90229	04734	59193
54164	58492	22421	74103	47070	25306	76468	26384	58151
32639	32363	05597	24200	13363	38005	94342	28728	35806
29334	27001	87637	87308	58731	00256	45834	15398	46557
02488	33062	28834	07351	19731	92420	60952	61280	50001
81525	72295	04839	96423	24878	82651	66566	14778	76797
29676	20591	68086	26432	46901	20849	89768	81536	86645
00742	57392	39064	66432	84673	40027	32832	61362	98947
05366	04213	25669	26422	44407	44048	37937	63904	45766
91921	26418	64117	94305	26766	25940	39972	22209	71500
00582	04711	87917	77341	42206	35126	74087	99547	81817
00725	69884	62797	56170	86324	88072	76222	36086	84637
69011	65795	95876	55293	18988	27354	26575	08625	40801
25976	57948	29888	88604	67917	48708	18912	82271	65424
09763	83473	73577	12908	30883	18317	28290	35797	05998
91567	42595	27958	30134	04024	86385	29880	99730	55536
17955	56349	90999	49127	20044	59931	06115	20542	18059
46503	18584	18845	49618	02304	51038	20655	58727	28168
92157	89634	94824	78171	84610	82834	09922	25417	44137
14577	62765	35605	81263	39667	47358	56873	56307	67607

[a] Reproduced with permission from *Probability and Statistics in Engineering and Management Science*, 3rd edition, by W. W. Hines and D. C. Montgomery, Wiley, New York, 1990.

XII. Alias Relationships for 2^{k-p} Fractional Factorial Designs with $k \leq 15$ and $n \leq 64$

Designs with 3 Factors

(a) 2^{3-1}; 1/2 fraction of 3 factors in 4 runs — **Resolution III**

Design Generators

$C = AB$

Defining relation: $I = ABC$

Aliases

$A = BC$

$B = AC$

$C = AB$

Designs with 4 Factors

(b) 2^{4-1}; 1/2 fraction of 4 factors in 8 runs — **Resolution IV**

Design Generators

$D = ABC$

Defining relation: $I = ABCD$

Aliases

$A = BCD$

$B = ACD$

$C = ABD$

$D = ABC$

$AB = CD$

$AC = BD$

$AD = BC$

Designs with 5 Factors

(c) 2^{5-2}; 1/4 fraction of 5 factors in 8 runs — **Resolution III**

Design Generators

$D = AB \quad E = AC$

Defining relation: $I = ABD = ACE = BCDE$

Aliases

$A = BD = CE$

$B = AD = CDE$

$C = AE = BDE$

$D = AB = BCE$

$E = AC = BCD$

$BC = DE = ACD = ABE$

$CD = BE = ABC = ADE$

(d) 2^{5-1}; 1/2 fraction of 5 factors in 16 runs — **Resolution V**

Design Generators

$E = ABCD$

Defining relation: $I = ABCDE$

Aliases

Each main effect is aliased with a single 4-factor interaction.

$AB = CDE \quad BD = ACE$

$AC = BDE \quad BE = ACD$

$AD = BCE \quad CD = ABE$

$AE = BCD \quad CE = ABD$

$BC = ADE \quad DE = ABC$

2 blocks of 8: $AB = CDE$

XII. Alias Relationships for 2^{k-p} Fractional Factorial Designs with $k \leq 15$ and $n \leq 64$ (*continued*)

Designs with 6 Factors

(e) 2^{6-3}; 1/8 fraction of 6 factors in 8 runs — **Resolution III**

Design Generators

$D = AB \quad E = AC \quad F = BC$

Defining relation: $I = ABD = ACE = BCDE = BCF = ACDF = ABEF = DEF$

Aliases

$A = BD = CE = CDF = BEF$	$E = AC = DF = BCD = ABF$
$B = AD = CF = CDE = AEF$	$F = BC = DE = ACD = ABE$
$C = AE = BF = BDE = ADF$	$CD = BE = AF = ABC = ADE = BDF = CEF$
$D = AB = EF = BCE = ACF$	

(f) 2^{6-2}; 1/4 fraction of 6 factors in 16 runs — **Resolution IV**

Design Generators

$E = ABC \quad F = BCD$

Defining relation: $I = ABCE = BCDF = ADEF$

Aliases

$A = BCE = DEF$	$AB = CE$
$B = ACE = CDF$	$AC = BE$
$C = ABE = BDF$	$AD = EF$
$D = BCF = AEF$	$AE = BC = DF$
$E = ABC = ADF$	$AF = DE$
$F = BCD = ADE$	$BD = CF$
$ABD = CDE = ACF = BEF$	$BF = CD$
$ACD = BDE = ABF = CEF$	

2 blocks of 8: $ABD = CDE = ACF = BEF$

(g) 2^{6-1}; 1/2 fraction of 6 factors in 32 runs — **Resolution VI**

Design Generators

$F = ABCDE$

Defining relation: $I = ABCDEF$

Aliases

Each main effect is aliased with a single 5-factor interaction.
Each 2-factor interaction is aliased with a single 4-factor interaction.

$ABC = DEF$ $\quad ACE = BDF$
$ABD = CEF$ $\quad ACF = BDE$
$ABE = CDF$ $\quad ADE = BCF$
$ABF = CDE$ $\quad ADF = BCE$
$ACD = BEF$ $\quad AEF = BCD$
2 blocks of 16: $ABC = DEF$ $\quad$ 4 blocks of 8: $AB = CDEF$
$ACD = BEF$
$AEF = BCD$

Designs with 7 Factors

(h) 2^{7-4}; 1/16 fraction of 7 factors in 8 runs — **Resolution III**

Design Generators

$D = AB \quad E = AC \quad F = BC \quad G = ABC$

Defining relation: $I = ABD = ACE = BCDE = BCF = ACDF = ABEF = DEF = ABCG$
$= CDG = BEG = ADEG = AFG = BDFG = CEFG = ABCDEFG$

Aliases

$A = BD = CE = FG$ $\quad E = AC = DF = BG$
$B = AD = CF = EG$ $\quad F = BC = DE = AG$
$C = AE = BF = DG$ $\quad G = CD = BE = AF$
$D = AB = EF = CG$

XII. Alias Relationships for 2^{k-p} Fractional Factorial Designs with $k \leq 15$ and $n \leq 64$ (*continued*)

(i) 2^{7-3}; 1/8 fraction of 7 factors in 16 runs — **Resolution IV**

Design Generators

$E = ABC \quad F = BCD \quad G = ACD$

Defining relation: $I = ABCE = BCDF = ADEF = ACDG = BDEG = ABFG = CEFG$

Aliases

$A = BCE = DEF = CDG = BFG$	$AB = CE = FG$	$E = ABC = ADF = BDG = CFG$	$AF = DE = BG$
$B = ACE = CDF = DEG = AFG$	$AC = BE = DG$	$F = BCD = ADE = ABG = CEG$	$AG = CD = BF$
$C = ABE = BDF = ADG = EFG$	$AD = EF = CG$	$G = ACD = BDE = ABF = CEF$	$BD = CF = EG$
$D = BCF = AEF = ACG = BEG$	$AE = BC = DF$		

$ABD = CDE = ACF = BEF = BCG = AEG = DFG$

2 blocks of 8: $ABD = CDE = ACF = BEF = BCG = AEG = DFG$

(j) 2^{7-2}; 1/4 fraction of 7 factors in 32 runs — **Resolution IV**

Design Generators

$F = ABCD \quad G = ABDE$

Defining relation: $I = ABCDF = ABDEG = CEFG$

Aliases

$A =$	$AB = CDF = DEG$	$BC = ADF$	$CE = FG$	$ACE = AFG$
$B =$	$AC = BDF$	$BD = ACF = AEG$	$CF = ABD = EG$	$ACG = AEF$
$C = EFG$	$AD = BCF = BEG$	$BE = ADG$	$CG = EF$	$BCE = BFG$
$D =$	$AE = BDG$	$BF = ACD$	$DE = ABG$	$BCG = BEF$
$E = CFG$	$AF = BCD$	$BG = ADE$	$DF = ABC$	$CDE = DFG$
$F = CEG$	$AG = BDE$	$CD = ABF$	$DG = ABE$	$CDG = DEF$
$G = CEF$				

2 blocks of 16: $ACE = AFG$

4 blocks of 8: $ACE = AFG$, $BCE = BFG$, $AB = CDF = DEG$

(k) 2^{7-1}; 1/2 fraction of 7 factors in 64 runs — **Resolution VII**

Design Generators

$G = ABCDEF$

Defining relation: $I = ABCDEFG$

Aliases

Each main effect is aliased with a single 6-factor interaction.
Each 2-factor interaction is aliased with a single 5-factor interaction.
Each 3-factor interaction is aliased with a single 4-factor interaction.

2 blocks of 32: ABC

4 blocks of 16: ABC, CEF, CDG

Designs with 8 Factors

(l) 2^{8-4}; 1/16 fraction of 8 factors in 16 runs — **Resolution IV**

Design Generators

$E = BCD \quad F = ACD \quad G = ABC \quad H = ABD$

Defining relation: $I = BCDE = ACDF = ABEF = ABCG = ADEG = BDFG = CEFG = ABDH = ACEH = BCFH = DEFH = CDGH = BEGH = AFGH = ABCDEFGH$

Aliases

$A = CDF = BEF = BCG = DEG = BDH = CEH = FGH$	$AB = EF = CG = DH$
$B = CDE = AEF = ACG = DFG = ADH = CFH = EGH$	$AC = DF = BG = EH$
$C = BDE = ADF = ABG = EFG = AEH = BFH = DGH$	$AD = CF = EG = BH$
$D = BCE = ACF = AEG = BFG = ABH = EFH = CGH$	$AE = BF = DG = CH$
$E = BCD = ABF = ADG = CFG = ACH = DFH = BGH$	$AF = CD = BE = GH$
$F = ACD = ABE = BDG = CEG = BCH = DEH = AGH$	$AG = BC = DE = FH$
$G = ABC = ADE = BDF = CEF = CDH = BEH = AFH$	$AH = BD = CE = FG$
$H = ABD = ACE = BCF = DEF = CDG = BEG = AFG$	

2 blocks of 8: $AB = EF = CG = DH$

XII. Alias Relationships for 2^{k-p} Fractional Factorial Designs with $k \leq 15$ and $n \leq 64$ (*continued*)

(m) 2^{8-3}; 1/8 fraction of 8 factors in 32 runs — **Resolution IV**

Design Generators

$F = ABC \quad G = ABD \quad H = BCDE$

Defining relation: $I = ABCF = ABDG = CDFG = BCDEH = ADEFH = ACEGH = BEFGH$

Aliases

$A = BCF = BDG$	$AE = DFH = CGH$	$DE = BCH = AFH$
$B = ACF = ADG$	$AF = BC = DEH$	$DH = BCE = AEF$
$C = ABF = DFG$	$AG = BD = CEH$	$EF = ADH = BGH$
$D = ABG = CFG$	$AH = DEF = CEG$	$EG = ACH = BFH$
$E =$	$BE = CDH = FGH$	$EH = BCD = ADF = ACG = BFG$
$F = ABC = CDG$	$BH = CDE = EFG$	$FH = ADE = BEG$
$G = ABD = CDF$	$CD = FG = BEH$	$GH = ACE = BEF$
$H =$	$CE = BDH = AGH$	$ABE = CEF = DEG$
$AB = CF = DG$	$CG = DF = AEH$	$ABH = CFH = DGH$
$AC = BF = EGH$	$CH = BDE = AEG$	$ACD = BDF = BCG = AFG$
$AD = BG = EFH$		

2 blocks of 16: $ABE = CEF = DEG$

4 blocks of 8: $ABE = CEF = DEG$, $ABH = CFH = DGH$, $EH = BCD = ADF = ACG = BFG$

(n) 2^{8-2}; 1/4 fraction of 8 factors in 64 runs

Design Generators

$G = ABCD \quad H = ABEF$

Defining relation: $I = ABCDG = ABEFH = CDEFGH$

Aliases

$AB = CDG = EFH$	$BG = ACD$	$EF = ABH$	$ADH =$	$BFG =$
$AC = BDG$	$BH = AEF$	$EG =$	$AEG =$	$BGH =$
$AD = BCG$	$CD = ABG$	$EH = ABF$	$AFG =$	$CDE = FGH$
$AE = BFH$	$CE =$	$FG =$	$AGH =$	$CDF = EGH$
$AF = BEH$	$CF =$	$FH = ABE$	$BCE =$	$CDH = EFG$
$AG = BCD$	$CG = ABD$	$GH =$	$BCF =$	$CEF = DGH$
$AH = BEF$	$CH =$	$ACE =$	$BCH =$	$CEG = DFH$
$BC = ADG$	$DE =$	$ACF =$	$BDE =$	$CEH = DFG$
$BD = ACG$	$DF =$	$ACH =$	$BDF =$	$CFG = DEH$
$BE = AFH$	$DG = ABC$	$ADE =$	$BDH =$	$CFH = DEG$
$BF = AEH$	$DH =$	$ADF =$	$BEG =$	$CGH = DEF$

2 blocks of 32: $CDE = FGH$ 4 blocks of 16: $CDE = FGH$
ACF
BDH

XII. Alias Relationships for 2^{k-p} Fractional Factorial Designs with $k \leq 15$ and $n \leq 64$ (*continued*)

Designs with 9 Factors

(o) 2^{9-5}; 1/32 fraction of 9 factors in 16 runs — **Resolution III**

Design Generators

$E = ABC \quad F = BCD \quad G = ACD \quad H = ABD \quad J = ABCD$

Defining relation: $I = ABCE = BCDF = ADEF = ACDG = BDEG = ABFG = CEFG = ABDH$
$= CDEH = ACFH = BEFH = BCGH = AEGH = DFGH = ABCDEFGH = ABCDJ$
$= DEJ = AFJ = BCEFJ = BGJ = ACEGJ = CDFGJ = ABDEFGJ = CHJ$
$= ABEHJ = BDFHJ = ABCDEFHJ = ADGHJ = BCDEFGHJ = ABCFGHJ = EFGHJ$

Aliases

$A = FJ$
$B = GJ$
$C = HJ$
$D = EJ$
$E = DJ$
$F = AJ$
$G = BJ$
$H = CJ$
$J = DE = AF = BG = CH$
$AB = CE = FG = DH$
$AC = BE = DG = FH$
$AD = EF = CG = BH$
$AE = BC = DF = GH$
$AG = CD = BF = EH$
$AH = BD = CF = EG$

2 blocks of 8: $AB = CE = FG = DH$

(p) 2^{9-4}; 1/16 fraction of 9 factors in 32 runs

Resolution IV

Design Generators

$F = BCDE \quad G = ACDE \quad H = ABDE \quad J = ABCE$

Defining relation: $I = BCDEF = ACDEG = ABFG = ABDEH = ACFH = BCGH = DEFGH = ABCEJ = ADFJ = BDGJ = CEFGJ = CDHJ = BEFHJ = AEGHJ = ABCDFGHJ$

Aliases

$A = BFG = CFH = DFJ$	$AD = CEG = BEH = FJ$	$BJ = ACE = DG = EFH$
$B = AFG = CGH = DGJ$	$AE = CDG = BDH = BCJ = GHJ$	$CD = BEF = AEG = HJ$
$C = AFH = BGH = DHJ$	$AF = BG = CH = DJ$	$CE = BDF = ADG = ABJ = FGJ$
$D = AFJ = BGJ = CHJ$	$AG = CDE = BF = EHJ$	$CJ = ABE = EFG = DH$
$E =$	$AH = BDE = CF = EGJ$	$DE = BCF = ACG = ABH = FGH$
$F = ABG = ACH = ADJ$	$AJ = BCE = DF = EGH$	$EF = BCD = DGH = CGJ = BHJ$
$G = ABF = BCH = BDJ$	$BC = DEF = GH = AEJ$	$EG = ACD = DFH = CFJ = AHJ$
$H = ACF = BCG = CDJ$	$BD = CEF = AEH = GJ$	$EH = ABD = DFG = BFJ = AGJ$
$J = ADF = BDG = CDH$	$BE = CDF = ADH = ACJ = FHJ$	$EJ = ABC = CFG = BFH = AGH$
$AB = FG = DEH = CEJ$	$BH = ADE = CG = EFJ$	$AEF = BEG = CEH = DEJ$
$AC = DEG = FH = BEJ$		

2 blocks of 16: $AEF = BEG = CEH = DEJ$

4 blocks of 8: $AEF = BEG = CEH = DEJ$
$AB = FG = DEH = CEJ$
$CD = BEF = AEG = HJ$

(q) 2^{9-3}; 1/8 fraction of 9 factors in 64 runs

Resolution IV

Design Generators

$G = ABCD \quad H = ACEF \quad J = CDEF$

Defining relation: $I = ABCDG = ACEFH = BDEFGH = CDEFJ = ABEFGJ = ADHJ = BCGHJ$

Aliases

$A = DHJ$	$AC = BDG = EFH$	$BF =$
$B =$	$AD = BCG = HJ$	$BG = ACD = CHJ$
$C =$	$AE = CFH$	$BH = CGJ$
$D = AHJ$	$AF = CEH$	$BJ = CGH$
$E =$	$AG = BCD$	$CD = ABG = EFJ$
$F =$	$AH = CEF = DJ$	$CE = AFH = DFJ$
$G =$	$AJ = DH$	$CF = AEH = DEJ$
$H = ADJ$	$BC = ADG = GHJ$	$CG = ABD = BHJ$
$J = ADH$	$BD = ACG$	$CH = AEF = BGJ$
$AB = CDG$	$BE =$	$CJ = DEF = BGH$
$DE = CFJ$	$GJ = BCH$	$AFJ = BEG = DFH$
$DF = CEJ$	$ABE = FGJ$	$AGH = DGJ$
$DG = ABC$	$ABF = EGJ$	$AGJ = BEF = DGH$
$EF = ACH = CDJ$	$ABH = BDJ$	$BCE =$
$EG =$	$ABJ = EFG = BDH$	$BCF =$
$EH = ACF$	$ACJ = CDH$	$BDE = FGH$
$EJ = CDF$	$ADE = EHJ$	$BDF = EGH$
$FG =$	$ADF = FHJ$	$BEH = DFG$
$FH = ACE$	$AEG = BFJ$	$BFH = DEG$
$FJ = CDE$	$AEJ = BFG = DEH$	$CEG =$
$GH = BCJ$	$AFG = BEJ$	$CFG =$

2 blocks of 32: CFG

4 blocks of 16: CFG
$AGJ = BEF = DGH$
$ADE = EHJ$

(r) 2^{10-6}; 1/64 fraction of 10 factors in 16 runs

Resolution III

Design Generators

$E = ABC \quad F = BCD \quad G = ACD \quad H = ABD \quad J = ABCD \quad K = AB$

Defining relation: $I = ABCE = BCDF = ADEF = ACDG = BDEG = ABFG = CEFG = ABDH$
$= CDEH = ACFH = BEFH = BCGH = AEGH = DFGH = ABCDEFGH = ABCDJ$
$= DEJ = AFJ = BCEFJ = BGJ = ACEGJ = CDFGI = ABDEFGJ = CHJ$
$= ABEHJ = BDFHJ = ACDEFHJ = ADGHJ = BCDEGHJ = ABCFGHJ = EFGHJ = ABK$
$= CEK = ACDFK = BDEFK = BCDGK = ADEGK = FGK = ABCEFGK = DHK$
$= ABCDEHK = BCFHK = AEFHK = ACGHK = BEGHK = ABDFGHK = CDEFGHK = CDJK$
$= ABDEJK = BFJK = ACEFJK = AGJK = BCEGJK = ABCDFGJK = DEFGJK = ABCHJK$
$= EHJK = ADFHJK = BCDEFHJK = BDGHJK = ACDEGHJK = CFGHJK = ABEFGHJK$

Aliases

$A = FJ = BK$	$J = DE = AF = BG = CH$
$B = GJ = AK$	$K = AB = CE = FG = DH$
$C = HJ = EK$	$AC = BE = DG = FH$
$D = EJ = HK$	$AD = EF = CG = BH$
$E = DJ = CK$	$AE = BC = DF = GH$
$F = AJ = GK$	$AG = CD = BF = EH = JK$
$G = BJ = FK$	$AH = BD = CF = EG$
$H = CJ = DK$	

2 blocks of 8: $AG = CD = BF = EH = JK$

XII. Alias Relationships for 2^{k-p} Fractional Factorial Designs with $k \leq 15$ and $n \leq 64$ (*continued*)

(s) 2^{10-5}; 1/32 fraction of 10 factors in 32 runs — **Resolution IV**

Design Generators

$F = ABCD \quad G = ABCE \quad H = ABDE \quad J = ACDE \quad K = BCDE$

Defining relation: $I = ABCDF = ABCEG = DEFG = ABDEH = CEFH = CDGH = ABFGH = ACDEJ$
$= BEFJ = BDGJ = ACFGJ = BCHJ = ADFHJ = AEGHJ = BCDEFGHJ = BCDEK$
$= AEFK = ADGK = BCFGK = ACHK = BDFHK = BEGHK = ACDEFGHK = ABJK$
$= CDFJK = CEGJK = ABDEFGJK = DEHJK = ABCEFHJK = ABCDGHJK = FGHJK$

Aliases

$A = EFK = DGK = CHK = BJK$	$AH = BDE = BFG = DFJ = EGJ = CK$
$B = EFJ = DGJ = CHJ = AJK$	$AJ = CDE = CFG = DFH = EGH = BK$
$C = EFH = DGH = BHJ = AHK$	$AK = EF = DG = CH = BJ$
$D = EFG = CGH = BGJ = AGK$	$BC = ADF = AEG = HJ = DEK = FGK$
$E = DFG = CFH = BFJ = AFK$	$BD = ACF = AEH = GJ = CEK = FHK$
$F = DEG = CEH = BEJ = AEK$	$BE = ACG = ADH = FJ = CDK = GHK$
$G = DEF = CDH = BDJ = ADK$	$BF = ACD = AGH = EJ = CGK = DHK$
$H = CEF = CDG = BCJ = ACK$	$BG = ACE = AFH = DJ = CFK = EHK$
$J = BEF = BDG = BCH = ABK$	$BH = ADE = AFG = CJ = DFK = EGK$
$K = AEF = ADG = ACH = ABJ$	$CD = ABF = GH = AEJ = BEK = FJK$
$AB = CDF = CEG = DEH = FGH = JK$	$CE = ABG = FH = ADJ = BDK = GJK$
$AC = BDF = BEG = DEJ = FGJ = HK$	$CF = ABD = EH = AGJ = BGK = DJK$
$AD = BCF = BEH = CEJ = FHJ = GK$	$CG = ABE = DH = AFJ = BFK = EJK$
$AE = BCG = BDH = CDJ = GHJ = FK$	$DE = FG = ABH = ACJ = BCK = HJK$
$AF = BCD = BGH = CGJ = DHJ = EK$	$DF = ABC = EG = AHJ = BHK = CJK$
$AG = BCE = BFH = CFJ = EHJ = DK$	

2 blocks of 16: $AK = EF = DG = CH = BJ$

4 blocks of 8: $AK = EF = DG = CH = BJ$
$AJ = CDE = CFG = DFH = EGH = BK$
$AB = CDF = CEG = DEH = FGH = JK$

(t) 2^{10-4}; 1/16 fraction of 10 factors in 64 runs

Resolution IV

Design Generators

$G = BCDF \quad H = ACDF \quad J = ABDE \quad K = ABCE$

Defining relation: $I = BCDFG = ACDFH = ABGH = ABDEJ = ACEFGJ = BCEFHJ = DEGHJ = ABCEK = ADEFGK = BDEFHK = CEGHK = CDJK = BFGJK = AFHJK = ABCDGHJK$

Aliases

$A = BGH$	$AD = CFH = BEJ$	$BK = ACE = FGJ$
$B = AGH$	$AE = BDJ = BCK$	$CD = BFG = AFH = JK$
$C = DJK$	$AF = CDH = HJK$	$CE = ABK = GHK$
$D = CJK$	$AG = BH$	$CF = BDG = ADH$
$E =$	$AH = CDF = BG = FJK$	$CG = BDF = EHK$
$F =$	$AJ = BDE = FHK$	$CH = ADF = EGK$
$G = ABH$	$AK = BCE = FHJ$	$CJ = DK$
$H = ABG$	$BC = DFG = AEK$	$CK = ABE = EGH = DJ$
$J = CDK$	$BD = CFG = AEJ$	$DE = ABJ = GHJ$
$K = CDJ$	$BE = ADJ = ACK$	$DF = BCG = ACH$
$AB = GH = DEJ = CEK$	$BF = CDG = GJK$	$DG = BCF = EHJ$
$AC = DFH = BEK$	$BJ = ADE = FGK$	$DH = ACF = EGJ$
$EF =$	$GJ = DEH = BFK$	$AEG = BEH = CFJ = DFK$
$EG = DHJ = CHK$	$GK = CEH = BFJ$	$AEH = BEG$
$EH = DGJ = CGK$	$HJ = DEG = AFK$	$AFG = BFH = CEJ = DEK$
$EJ = ABD = DGH$	$HK = CEG = AFJ$	$AGJ = CEF = BHJ$
$EK = ABC = CGH$	$ABF = FGH$	$AGK = DEF = BHK$
$FG = BCD = BJK$	$ACG = BCH = EFJ$	$BCJ = EFH = BDK$
$FH = ACD = AJK$	$ACJ = EFG = ADK$	$BEF = CHJ = DHK$
$FJ = BGK = AHK$	$ADG = BDH = EFK$	$CDE = EJK$
$FK = BGJ = AHJ$	$AEF = CGJ = DGK$	$CFK = DFJ$

2 blocks of 32: $AGJ = CEF = BHJ$

4 blocks of 16: $AGJ = CEF = BHJ$
$AGK = DEF = BHK$
$CD = BFG = AFH = JK$

XII. Alias Relationships for 2^{k-p} Fractional Factorial Designs with $k \leq 15$ and $n \leq 64$ (*continued*)

Desgins with 11 Factors

(u) 2^{11-7}; 1/128 fraction of 11 factors in 16 runs — **Resolution III**

Design Generators

$$E = ABC \quad F = BCD \quad G = ACD \quad H = ABD \quad J = ABCD \quad K = AB \quad L = AC$$

Defining relation:
$$\begin{aligned} I &= ABCE = BCDF = ADEF = ACDG = BDEG = ABFG = CEFG = ABDH \\ &= CDEH = ACFH = BEFH = BCGH = AEGH = DFGH = ABCDEFGH = ABCDJ \\ &= DEJ = AFJ = BCEFJ = BGJ = ACEGJ = CDFGJ = ABDEFGJ = CHJ \\ &= ABEHJ = BDFHJ = ACDEFHJ = ADGHJ = BCDEGHJ = ABCFGHJ = EFGHJ = ABK \\ &= CEK = ACDFK = BDEFK = BCDGK = ADEGK = FGK = ABCEFGK = DHK \\ &= ABCDEHK = BCFHK = AEFHK = ACGHK = BEGHK = ABDFGHK = CDEFGHK = CDJK \\ &= ABDEJK = BFJK = ACEFJK = AGJK = BCEGJK = ABCDFGJK = DEFGJK = ABCHJK \\ &= EHJK = ADFHJK = BCDEFHJK = BDGHJK = ACDEGHJK = CFGHJK = ABEFGHJK = ACL \\ &= BEL = ABDFL = CDEFL = DGL = ABCDEGL = BCFGL = AEFGL = BCDHL \\ &= ADEHL = FHL = ABCEFHL = ABGHL = CEGHL = ACDFGHL = BDEFGHL = BDJL \\ &= ACDEJL = CFJL = ABEFJL = ABCGJL = EGJL = ADFGJL = BCDEFGJL = AHJL \\ &= BCEHJL = ABCDFHJL = DEFHJL = CDGHJL = ABDEGHJL = BFGHJL = ACEFGHJL = BCKL \\ &= AEKL = DFKL = ABCDEFKL = ABDGKL = CDEGKL = ACFGKL = BEFGKL = ACDHKL \\ &= BDEHKL = ABFHKL = CEFHKL = GHKL = ABCEGHKL = BCDFGHKL = ADEFGHKL = ADJKL \\ &= BCDEJKL = ABCFJKL = EFJKL = CGJKL = ABEGJKL = BDFGJKL = ACDEFGJKL = BHJKL \\ &= ACEHJKL = CDFHJKL = ABDEFHJKL = ABCDGHJKL = DEGHJKL = AFGHJKL = BCEFGHJKL \end{aligned}$$

Aliases

$A = FJ = BK = CL$	$J = DE = AF = BG = CH$
$B = GJ = AK = EL$	$K = AB = CE = FG = DH$
$C = HJ = EK = AL$	$L = AC = BE = DG = FH$
$D = EJ = HK = GL$	$AD = EF = CG = BH$
$E = DJ = CK = BL$	$AE = BC = DF = GH = KL$
$F = AJ = GK = HL$	$AG = CD = BF = EH = JK$
$G = BJ = FK = DL$	$AH = BD = CF = EG = JL$
$H = CJ = DK = FL$	

2 blocks of 8: $AE = BC = DF = GH = KL$

(v) 2^{11-6}; 1/64 fraction of
11 factors in 32 runs

Resolution IV

Design Generators

$$F = ABC \quad G = BCD \quad H = CDE \quad J = ACD \quad K = ADE \quad L = BDE$$

Defining relation: $I = ABCF = BCDG = ADFG = CDEH = ABDEFH = BEGH = ACEFGH = ACDJ = BDFJ = ABGJ = CFGJ$
$= AEHJ = BCEFHJ = ABCDEGHJ = DEFGHJ = ADEK = BCDEFK = ABCEGK = EFGK = ACHK = BFHK$
$= ABDGHK = CDFGHK = CEJK = ABEFJK = BDEGJK = ACDEFGJK = DHJK = ABCDFHJK = BCGHJK$
$= AFGHJK = BDEL = ACDEFL = CEGL = ABEFGL = BCHL = AFHL = DGHL = ABCDFGHL$
$= ABCEJL = EFJL = ADEGJL = BCDEFGJL = ABDHJL = CDFHJL = ACGHJL = BFGHJL = ABKL$
$= CFKL = ACDGKL = BDFGKL = ABCDEHKL = DEFHKL = AEGHKL = BCEFGHKL = BCDJKL$
$= ADFJKL = GJKL = ABCFGJKL = BEHJKL = ACEFHJKL = CDEGHJKL = ABDEFGHJKL$

Aliases

$A = BCF = DFG = CDJ = BGJ = EHJ = DEK = CHK = FHL = BKL$
$B = ACF = CDG = EGH = DFJ = AGJ = FHK = DEL = CHL = AKL$
$C = ABF = BDG = DEH = ADJ = FGJ = AHK = EJK = EGL = BHL = FKL$
$D = BCG = AFG = CEH = ACJ = BFJ = AEK = HJK = BEL = GHL$
$E = CDH = BGH = AHJ = ADK = FGK = CJK = BDL = CGL = FJL$
$F = ABC = ADG = BDJ = CGJ = EGK = BHK = AHL = EJL = CKL$
$G = BCD = ADF = BEH = ABJ = CFJ = EFK = CEL = DHL = JKL$
$H = CDE = BEG = AEJ = ACK = BFK = DJK = BCL = AFL = DGL$
$J = ACD = BDF = ABG = CFG = AEH = CEK = DHK = EFL = GKL$
$K = ADE = EFG = ACH = BFH = CEJ = DHJ = ABL = CFL = GJL$
$L = BDE = CEG = BCH = AFH = DGH = EFJ = ABK = CFK = GJK$

$AB = CF = GJ = KL \quad AE = HJ = DK \quad AH = EJ = CK = FL \quad AL = FH = BK \quad BH = EG = CL = FK$
$AC = BF = DJ = HK \quad AF = BC = DG = HL \quad AJ = CD = BG = EH \quad BD = CG = FJ = EL \quad CE = DH = JK = GL$
$AD = FG = CJ = EK \quad AG = DF = BJ \quad AK = DE = CH = BL \quad BE = GH = DL \quad EF = GK = JL$

$ABD = CDF = ACG = BFG = EFH = BCJ = AFJ = DGJ = BEK = GHK = AEL = HJL = DKL$
$ABE = CEF = DFH = AGH = EGJ = BHJ = BDK = CGK = FJK = ADL = FGL = CJL = EKL$
$ABH = DEF = AEG = CFH = BEJ = GHJ = BCK = AFK = DGK = ACL = BFL = DJL = HKL$
$ACE = BEF = ADH = FGH = DEJ = CHJ = CDK = BGK = EHK = AJK = DFL = AGL = BJL$
$AEF = BCE = DEG = BDH = CGH = FHJ = DFK = AGK = BJK = CDL = BGL = EHL = AJL$

2 blocks of 16: $AB = CF = GJ = KL$

4 blocks of 8: $AB = CF = GJ = KL$
$AD = FG = CJ = EK$
$BD = CG = FJ = EL$

XII. Alias Relationships for 2^{k-p} Fractional Factorial Designs with $k \leq 15$ and $n \leq 64$ (*continued*)

Designs with 12 Factors

(w) 2^{12-8}; 1/256 fraction of 12 factors in 16 runs — **Resolution III**

Design Generators

$$E = ABC \quad F = ABD \quad G = ACD \quad H = BCD$$
$$J = ABCD \quad K = AB \quad L = AC \quad M = AD$$

Aliases

$$A = HJ = BK = CL = DM$$
$$B = GJ = AK = EL = FM$$
$$C = FJ = EK = AL = GM$$
$$D = EJ = FK = GL = AM$$
$$E = DJ = CK = BL = HM$$
$$F = CJ = DK = HL = BM$$
$$G = BJ = HK = DL = CM$$
$$H = AJ = GK = FL = EM$$
$$J = DE = CF = BG = AH$$
$$K = AB = CE = DF = GH$$
$$L = AC = BE = DG = FH$$
$$M = AD = BF = CG = EH$$
$$AE = BC = FG = DH = KL = JM$$
$$AF = BD = EG = CH = JL = KM$$
$$AG = EF = CD = BH = JK = LM$$

2 blocks of 8: $AE = BC = FG = DH = KL = JM$

Designs with 13 Factors

(x) 2^{13-9}; 1/512 fraction of 13 factors in 16 runs — **Resolution III**

Design Generators

$$E = ABC \quad F = ABD \quad G = ACD \quad H = BCD$$
$$J = ABCD \quad K = AB \quad L = AC \quad M = AD \quad N = BC$$

Aliases

$$A = HJ = BK = CL = DM = EN$$
$$B = GJ = AK = EL = FM = CN$$
$$C = FJ = EK = AL = GM = BN$$
$$D = EJ = FK = GL = AM = HN$$
$$E = DJ = CK = BL = HM = AN$$
$$F = CJ = DK = HL = BM = GN$$
$$G = BJ = HK = DL = CM = FN$$
$$H = AJ = GK = FL = EM = DN$$
$$J = DE = CF = BG = AH = MN$$
$$K = AB = CE = DF = GH = LN$$
$$L = AC = BE = DG = FH = KN$$
$$M = AD = BF = CG = EH = JN$$
$$N = BC = AE = FG = DH = KL = JM$$
$$AF = BD = EG = CH = JL = KM$$
$$AG = EF = CD = BH = JK = LM$$

2 blocks of 8: $AF = BD = EG = CH = JL = KM$

XII. Alias Relationships for 2^{k-p} Fractional Factorial Designs with $k \leq 15$ and $n \leq 64$ (*continued*)

Designs with 14 Factors

(y) 2^{14-10}; 1/1024 fraction of 14 factors in 16 runs — **Resolution III**

Design Generators

$E = ABC \quad F = ABD \quad G = ACD \quad H = BCD \quad J = ABCD$
$K = AB \quad L = AC \quad M = AD \quad N = BC \quad O = BD$

Aliases

$A = HJ = BK = CL = DM = EN = FO$
$B = GJ = AK = EL = FM = CN = DO$
$C = FJ = EK = AL = GM = BN = HO$
$D = EJ = FK = GL = AM = HN = BO$
$E = DJ = CK = BL = HM = AN = GO$
$F = CJ = DK = HL = BM = GN = AO$
$G = BJ = HK = DL = CM = FN = EO$
$H = AJ = GK = FL = EM = DN = CO$
$J = DE = CF = BG = AH = MN = LO$
$K = AB = CE = DF = GH = LN = MO$
$L = AC = BE = DG = FH = KN = JO$
$M = AD = BF = CG = EH = JN = KO$
$N = BC = AE = FG = DH = KL = JM$
$O = BD = AF = EG = CH = JL = KM$
$AG = EF = CD = BH = JK = LM = NO$

2 blocks of 8: $AG = EF = CD = BH = JK = LM = NO$

Designs with 15 Factors

(z) 2^{15-11}; 1/2048 fraction of 15 factors in 16 runs — **Resolution III**

Design Generators

$E = ABC \quad F = ABD \quad G = ACD \quad H = BCD \quad J = ABCD$
$K = AB \quad L = AC \quad M = AD \quad N = BC \quad O = BD \quad P = CD$

Aliases

$A = HJ = BK = CL = DM = EN = FO = GP$
$B = GJ = AK = EL = FM = CN = DO = HP$
$C = FJ = EK = AL = GM = BN = HO = DP$
$D = EJ = FK = GL = AM = HN = BO = CP$
$E = DJ = CK = BL = HM = AN = GO = FP$
$F = CJ = DK = HL = BM = GN = AO = EP$
$G = BJ = HK = DL = CM = FN = EO = AP$
$H = AJ = GK = FL = EM = DN = CO = BP$
$J = DE = CF = BG = AH = MN = LO = KP$
$K = AB = CE = DF = GH = LN = MO = JP$
$L = AC = BE = DG = FH = KN = JO = MP$
$M = AD = BF = CG = EH = JN = KO = LP$
$N = BC = AE = FG = DH = KL = JM = OP$
$O = BD = AF = EG = CH = JL = KM = NP$
$P = CD = EF = AG = BH = JK = LM = NO$

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